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Figure 1A – 1

	Atom Type		Resid	#	X	Y	Z	Occ	B		Mol		
ATOM	1	N	ILE	A	358	27.795	8.456	9.281	0.00	20.00	A	N	
ANISOU	1	N	ILE	A	358	2533	2533	2533	0	0	0	A	N
ATOM	3	CA	ILE	A	358	26.422	8.756	8.893	0.00	20.00	A	C	
ANISOU	3	CA	ILE	A	358	2533	2533	2533	0	0	0	A	C
ATOM	5	CB	ILE	A	358	26.425	9.191	7.426	0.00	20.00	A	C	
ANISOU	5	CB	ILE	A	358	2533	2533	2533	0	0	0	A	C
ATOM	7	CG1	ILE	A	358	25.062	9.773	7.044	0.00	20.00	A	C	
ANISOU	7	CG1	ILE	A	358	2533	2533	2533	0	0	0	A	C
ATOM	10	CD1	ILE	A	358	24.632	9.370	5.632	0.00	20.00	A	C	
ANISOU	10	CD1	ILE	A	358	2533	2533	2533	0	0	0	A	C
ATOM	14	CG2	ILE	A	358	26.688	7.974	6.520	0.00	20.00	A	C	
ANISOU	14	CG2	ILE	A	358	2533	2533	2533	0	0	0	A	C
ATOM	18	C	ILE	A	358	25.509	7.541	9.074	0.00	20.00	A	C	
ANISOU	18	C	ILE	A	358	2533	2533	2533	0	0	0	A	C
ATOM	19	O	ILE	A	358	24.403	7.625	9.592	0.00	20.00	A	O	
ANISOU	19	O	ILE	A	358	2533	2533	2533	0	0	0	A	O
ATOM	22	N	ARG	A	359	26.005	6.427	8.935	1.00	50.36	A	N	
ANISOU	22	N	ARG	A	359	6380	6367	6386	-8	-3	-4	A	N
ATOM	24	CA	ARG	A	359	25.428	5.111	8.655	1.00	50.29	A	C	
ANISOU	24	CA	ARG	A	359	6370	6362	6375	3	-3	0	A	C
ATOM	26	CB	ARG	A	359	24.390	5.087	7.515	1.00	50.51	A	C	
ANISOU	26	CB	ARG	A	359	6390	6404	6396	4	-10	5	A	C
ATOM	29	CG	AARG	A	359	23.442	3.867	7.558	0.50	51.02	A	C	
ANISOU	29	CG	AARG	A	359	6466	6445	6471	-7	12	-1	A	C
ATOM	30	CG	BARG	A	359	23.350	4.020	7.579	0.50	50.34	A	C	
ANISOU	30	CG	BARG	A	359	6379	6376	6369	4	0	-1	A	C
ATOM	35	CD	AARG	A	359	22.386	3.826	6.448	0.50	51.88	A	C	
ANISOU	35	CD	AARG	A	359	6569	6591	6550	-6	-10	-11	A	C
ATOM	36	CD	BARG	A	359	22.249	4.229	6.543	0.50	50.29	A	C	
ANISOU	36	CD	BARG	A	359	6380	6361	6366	3	5	-3	A	C
ATOM	41	NE	AARG	A	359	21.835	5.151	6.189	0.50	52.67	A	N	
ANISOU	41	NE	AARG	A	359	6663	6656	6690	26	3	-2	A	N
ATOM	42	NE	BARG	A	359	21.321	5.337	6.813	0.50	50.33	A	N	
ANISOU	42	NE	BARG	A	359	6376	6358	6388	-4	-7	15	A	N
ATOM	45	CZ	AARG	A	359	21.998	5.838	5.062	0.50	53.30	A	C	
ANISOU	45	CZ	AARG	A	359	6751	6760	6737	3	4	10	A	C
ATOM	46	CZ	BARG	A	359	21.200	6.448	6.076	0.50	50.04	A	C	
ANISOU	46	CZ	BARG	A	359	6346	6335	6331	5	-2	0	A	C
ATOM	47	NH1AARG	A	359	22.689	5.330	4.047	0.50	53.46	A	N		
ANISOU	47	NH1AARG	A	359	6767	6786	6757	5	3	-9	A	N	
ATOM	48	NH1BARG	A	359	21.980	6.674	5.019	0.50	50.01	A	N		
ANISOU	48	NH1BARG	A	359	6331	6324	6345	-1	1	0	A	N	
ATOM	53	NH2AARG	A	359	21.458	7.045	4.948	0.50	53.66	A	N		
ANISOU	53	NH2AARG	A	359	6794	6778	6814	8	-2	8	A	N	
ATOM	54	NH2BARG	A	359	20.295	7.359	6.415	0.50	49.97	A	N		
ANISOU	54	NH2BARG	A	359	6323	6360	6302	17	6	6	A	N	
ATOM	59	C	ARG	A	359	26.193	3.819	8.926	1.00	49.86	A	C	
ANISOU	59	C	ARG	A	359	6324	6319	6300	2	-2	2	A	C
ATOM	60	O	ARG	A	359	26.813	3.270	8.012	1.00	50.25	A	O	
ANISOU	60	O	ARG	A	359	6360	6373	6359	24	21	-10	A	O
ATOM	61	N	PRO	A	360	26.217	3.375	10.178	0.60	49.06	A	N	
ANISOU	61	N	PRO	A	360	6212	6208	6219	4	-1	-3	A	N
ATOM	62	CA	PRO	A	360	26.921	2.137	10.502	0.60	48.50	A	C	
ANISOU	62	CA	PRO	A	360	6150	6139	6139	-6	-6	-7	A	C
ATOM	64	CB	PRO	A	360	26.533	1.853	11.958	0.60	48.52	A	C	
ANISOU	64	CB	PRO	A	360	6149	6143	6144	0	-2	-7	A	C
ATOM	67	CG	PRO	A	360	25.611	2.936	12.384	0.60	48.68	A	C	
ANISOU	67	CG	PRO	A	360	6169	6164	6163	1	-5	-16	A	C
ATOM	70	CD	PRO	A	360	25.623	4.014	11.360	0.60	48.98	A	C	
ANISOU	70	CD	PRO	A	360	6214	6199	6194	1	-5	0	A	C

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Figure 1A - 2

ATOM	73	C	PRO A 360	26.429	1.021	9.602	0.60	47.92		A	C
ANISOU	73	C	PRO A 360	6077	6061	6067	11	0	0	A	C
ATOM	74	O	PRO A 360	25.459	1.186	8.862	0.60	48.07		A	O
ANISOU	74	O	PRO A 360	6106	6070	6086	11	-7	-7	A	O
ATOM	75	N	LYS A 361	27.085	-0.122	9.681	0.60	47.22		A	N
ANISOU	75	N	LYS A 361	5979	5989	5972	0	-8	-8	A	N
ATOM	77	CA	LYS A 361	26.709	-1.252	8.855	0.60	46.62		A	C
ANISOU	77	CA	LYS A 361	5899	5915	5900	1	6	0	A	C
ATOM	79	CB	LYS A 361	27.922	-2.138	8.598	0.60	46.63		A	C
ANISOU	79	CB	LYS A 361	5904	5910	5903	3	-2	-2	A	C
ATOM	82	CG	LYS A 361	29.242	-1.484	8.967	0.60	46.40		A	C
ANISOU	82	CG	LYS A 361	5879	5873	5878	5	-9	-3	A	C
ATOM	85	CD	LYS A 361	30.361	-2.492	9.024	0.60	46.34		A	C
ANISOU	85	CD	LYS A 361	5862	5864	5878	-9	-2	-9	A	C
ATOM	88	CE	LYS A 361	31.715	-1.812	9.071	0.60	46.17		A	C
ANISOU	88	CE	LYS A 361	5840	5850	5852	9	5	9	A	C
ATOM	91	NZ	LYS A 361	32.818	-2.797	9.273	0.60	45.89		A	N
ANISOU	91	NZ	LYS A 361	5833	5806	5797	0	-15	20	A	N
ATOM	95	C	LYS A 361	25.633	-2.060	9.558	0.60	46.19		A	C
ANISOU	95	C	LYS A 361	5852	5859	5838	2	0	-4	A	C
ATOM	96	O	LYS A 361	24.803	-2.695	8.911	0.60	45.83		A	O
ANISOU	96	O	LYS A 361	5808	5820	5785	7	3	-22	A	O
ATOM	97	N	GLU A 362	25.633	-2.000	10.889	1.00	45.71		A	N
ANISOU	97	N	GLU A 362	5778	5800	5788	4	3	7	A	N
ATOM	99	CA	GLU A 362	24.699	-2.787	11.700	1.00	45.40		A	C
ANISOU	99	CA	GLU A 362	5737	5760	5751	8	0	2	A	C
ATOM	101	CB	GLU A 362	25.078	-2.728	13.181	1.00	45.66		A	C
ANISOU	101	CB	GLU A 362	5784	5796	5765	5	0	0	A	C
ATOM	104	CG	AGLU A 362	26.298	-3.555	13.538	0.50	46.09		A	C
ANISOU	104	CG	AGLU A 362	5816	5848	5846	16	1	5	A	C
ATOM	105	CG	BGLU A 362	26.397	-3.417	13.501	0.50	45.86		A	C
ANISOU	105	CG	BGLU A 362	5794	5823	5805	14	0	4	A	C
ATOM	110	CD	AGLU A 362	26.700	-3.399	14.989	0.50	46.72		A	C
ANISOU	110	CD	AGLU A 362	5934	5940	5874	0	-10	-12	A	C
ATOM	111	CD	BGLU A 362	27.607	-2.591	13.073	0.50	45.96		A	C
ANISOU	111	CD	BGLU A 362	5832	5817	5813	-7	-7	0	A	C
ATOM	112	OE1AGLU A 362		27.907	-3.199	15.242	0.50	47.04		A	O
ANISOU	112	OE1AGLU A 362		5960	5991	5922	-32	0	-18	A	O
ATOM	113	OE1BGLU A 362		27.566	-1.353	13.227	0.50	45.81		A	O
ANISOU	113	OE1BGLU A 362		5791	5807	5805	14	-29	12	A	O
ATOM	114	OE2AGLU A 362		25.813	-3.477	15.871	0.50	47.09		A	O
ANISOU	114	OE2AGLU A 362		5954	5939	5998	-20	18	-5	A	O
ATOM	115	OE2BGLU A 362		28.598	-3.176	12.578	0.50	46.24		A	O
ANISOU	115	OE2BGLU A 362		5833	5885	5850	-5	19	16	A	O
ATOM	116	C	GLU A 362	23.246	-2.373	11.533	1.00	44.34		A	C
ANISOU	116	C	GLU A 362	5631	5616	5599	3	10	14	A	C
ATOM	117	O	GLU A 362	22.347	-3.010	12.092	1.00	45.03		A	O
ANISOU	117	O	GLU A 362	5693	5717	5699	-15	28	-1	A	O
ATOM	118	N	VAL A 363	23.009	-1.329	10.749	1.00	42.81		A	N
ANISOU	118	N	VAL A 363	5390	5451	5424	15	13	-29	A	N
ATOM	120	CA	VAL A 363	21.655	-0.860	10.517	1.00	41.29		A	C
ANISOU	120	CA	VAL A 363	5236	5252	5198	-17	-3	-42	A	C
ATOM	122	CB	VAL A 363	21.632	0.640	10.212	1.00	41.51		A	C
ANISOU	122	CB	VAL A 363	5245	5272	5255	-7	1	-18	A	C
ATOM	124	CG1	VAL A 363	22.177	0.916	8.826	1.00	41.95		A	C
ANISOU	124	CG1	VAL A 363	5345	5315	5279	-18	-13	-25	A	C
ATOM	128	CG2	VAL A 363	20.233	1.173	10.350	1.00	42.19		A	C
ANISOU	128	CG2	VAL A 363	5329	5328	5373	24	-15	-34	A	C
ATOM	132	C	VAL A 363	21.034	-1.628	9.361	1.00	39.41		A	C
ANISOU	132	C	VAL A 363	4964	5026	4983	15	38	-56	A	C
ATOM	133	O	VAL A 363	19.820	-1.670	9.216	1.00	39.04		A	O
ANISOU	133	O	VAL A 363	4925	5029	4878	-14	36	-113	A	O

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Figure 1A – 3

ATOM	134	N	TYR	A	364	21.887	-2.234	8.543	1.00	37.42	A	N	
ANISOU	134	N	TYR	A	364	4722	4783	4713	-43	-2	-59	A	N
ATOM	136	CA	TYR	A	364	21.445	-3.013	7.393	1.00	35.61	A	C	
ANISOU	136	CA	TYR	A	364	4507	4519	4504	-14	33	-16	A	C
ATOM	138	CB	TYR	A	364	22.558	-3.033	6.351	1.00	36.02	A	C	
ANISOU	138	CB	TYR	A	364	4527	4608	4549	9	37	-44	A	C
ATOM	141	CG	TYR	A	364	22.782	-1.688	5.712	1.00	37.88	A	C	
ANISOU	141	CG	TYR	A	364	4850	4794	4749	8	84	9	A	C
ATOM	142	CD1	TYR	A	364	21.835	-1.149	4.859	1.00	39.14	A	C	
ANISOU	142	CD1	TYR	A	364	4916	5020	4933	30	23	-15	A	C
ATOM	144	CE1	TYR	A	364	22.026	0.083	4.266	1.00	41.16	A	C	
ANISOU	144	CE1	TYR	A	364	5233	5186	5218	-2	5	31	A	C
ATOM	146	CZ	TYR	A	364	23.177	0.801	4.525	1.00	42.25	A	C	
ANISOU	146	CZ	TYR	A	364	5306	5351	5396	-28	-45	30	A	C
ATOM	147	OH	TYR	A	364	23.353	2.033	3.925	1.00	43.76	A	O	
ANISOU	147	OH	TYR	A	364	5535	5450	5641	-37	6	72	A	O
ATOM	149	CE2	TYR	A	364	24.141	0.288	5.377	1.00	41.74	A	C	
ANISOU	149	CE2	TYR	A	364	5311	5236	5310	-19	-21	34	A	C
ATOM	151	CD2	TYR	A	364	23.935	-0.951	5.971	1.00	40.26	A	C	
ANISOU	151	CD2	TYR	A	364	5057	5107	5131	-48	-11	-24	A	C
ATOM	153	C	TYR	A	364	21.089	-4.435	7.783	1.00	33.15	A	C	
ANISOU	153	C	TYR	A	364	4158	4281	4153	0	20	-36	A	C
ATOM	154	O	TYR	A	364	21.930	-5.191	8.216	1.00	33.64	A	O	
ANISOU	154	O	TYR	A	364	4156	4308	4315	-22	48	-47	A	O
ATOM	155	N	LEU	A	365	19.836	-4.800	7.600	1.00	30.40	A	N	
ANISOU	155	N	LEU	A	365	3891	3878	3781	14	65	-43	A	N
ATOM	157	CA	LEU	A	365	19.359	-6.111	7.970	1.00	28.93	A	C	
ANISOU	157	CA	LEU	A	365	3685	3711	3596	32	40	-66	A	C
ATOM	159	CB	LEU	A	365	17.922	-6.001	8.456	1.00	28.24	A	C	
ANISOU	159	CB	LEU	A	365	3575	3616	3538	30	25	-57	A	C
ATOM	162	CG	LEU	A	365	17.759	-5.023	9.609	1.00	27.57	A	C	
ANISOU	162	CG	LEU	A	365	3444	3507	3521	-14	12	-54	A	C
ATOM	164	CD1	LEU	A	365	16.296	-4.986	10.037	1.00	27.71	A	C	
ANISOU	164	CD1	LEU	A	365	3494	3580	3454	80	84	-77	A	C
ATOM	168	CD2	LEU	A	365	18.658	-5.426	10.762	1.00	27.43	A	C	
ANISOU	168	CD2	LEU	A	365	3455	3537	3429	19	90	-105	A	C
ATOM	172	C	LEU	A	365	19.407	-7.080	6.796	1.00	27.95	A	C	
ANISOU	172	C	LEU	A	365	3580	3575	3462	16	48	-37	A	C
ATOM	173	O	LEU	A	365	19.421	-6.671	5.641	1.00	28.13	A	O	
ANISOU	173	O	LEU	A	365	3558	3652	3477	11	50	-6	A	O
ATOM	174	N	ASP	A	366	19.410	-8.357	7.131	1.00	27.17	A	N	
ANISOU	174	N	ASP	A	366	3476	3529	3317	21	73	-83	A	N
ATOM	176	CA	ASP	A	366	19.466	-9.445	6.171	1.00	26.45	A	C	
ANISOU	176	CA	ASP	A	366	3397	3366	3286	19	27	-54	A	C
ATOM	178	CB	ASP	A	366	20.255	-10.582	6.821	1.00	26.90	A	C	
ANISOU	178	CB	ASP	A	366	3463	3455	3303	72	26	-43	A	C
ATOM	181	CG	ASP	A	366	20.521	-11.736	5.888	1.00	28.73	A	C	
ANISOU	181	CG	ASP	A	366	3750	3631	3534	108	0	-101	A	C
ATOM	182	OD1	ASP	A	366	19.882	-11.822	4.810	1.00	30.70	A	O	
ANISOU	182	OD1	ASP	A	366	3973	4053	3639	113	-24	-234	A	O
ATOM	183	OD2	ASP	A	366	21.343	-12.625	6.194	1.00	30.56	A	O	
ANISOU	183	OD2	ASP	A	366	3934	3996	3681	269	6	-113	A	O
ATOM	184	C	ASP	A	366	18.056	-9.889	5.788	1.00	25.93	A	C	
ANISOU	184	C	ASP	A	366	3347	3332	3171	61	28	-18	A	C
ATOM	185	O	ASP	A	366	17.279	-10.369	6.620	1.00	25.20	A	O	
ANISOU	185	O	ASP	A	366	3330	3259	2986	88	102	-97	A	O
ATOM	186	N	ARG	A	367	17.706	-9.696	4.518	1.00	24.31	A	N	
ANISOU	186	N	ARG	A	367	3151	3196	2889	83	59	-78	A	N
ATOM	188	CA	ARG	A	367	16.371	-10.047	4.050	1.00	24.19	A	C	
ANISOU	188	CA	ARG	A	367	3119	3168	2903	50	61	-37	A	C
ATOM	190	CB	ARG	A	367	16.237	-9.748	2.549	1.00	23.77	A	C	
ANISOU	190	CB	ARG	A	367	3051	3083	2894	82	28	-30	A	C

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Figure 1A – 4

ATOM	193	CG	ARG A 367	14.856	-10.019	1.976	1.00	23.50		A	C
ANISOU	193	CG	ARG A 367	3133	2994	2800	8	41	0	A	C
ATOM	196	CD	ARG A 367	13.756	-9.175	2.614	1.00	23.67		A	C
ANISOU	196	CD	ARG A 367	2989	3058	2947	67	68	7	A	C
ATOM	199	NE	ARG A 367	12.468	-9.457	2.000	1.00	22.34		A	N
ANISOU	199	NE	ARG A 367	3178	2794	2515	24	-3	-171	A	N
ATOM	201	CZ	ARG A 367	11.621	-10.357	2.446	1.00	24.53		A	C
ANISOU	201	CZ	ARG A 367	3188	3129	3001	-12	59	-70	A	C
ATOM	202	NH1	ARG A 367	11.906	-11.077	3.535	1.00	24.45		A	N
ANISOU	202	NH1	ARG A 367	3364	3011	2913	6	10	-125	A	N
ATOM	205	NH2	ARG A 367	10.482	-10.550	1.813	1.00	26.56		A	N
ANISOU	205	NH2	ARG A 367	3480	3476	3132	-11	-68	-30	A	N
ATOM	208	C	ARG A 367	15.984	-11.493	4.344	1.00	24.00		A	C
ANISOU	208	C	ARG A 367	3104	3187	2829	75	23	-48	A	C
ATOM	209	O	ARG A 367	14.827	-11.791	4.605	1.00	23.53		A	O
ANISOU	209	O	ARG A 367	3133	3172	2632	28	-39	-59	A	O
ATOM	210	N	LYS A 368	16.944	-12.415	4.333	1.00	25.00		A	N
ANISOU	210	N	LYS A 368	3251	3270	2977	90	70	-21	A	N
ATOM	212	CA	LYS A 368	16.579	-13.789	4.547	1.00	25.77		A	C
ANISOU	212	CA	LYS A 368	3334	3308	3148	63	57	-38	A	C
ATOM	214	CB	LYS A 368	17.684	-14.740	4.067	1.00	26.57		A	C
ANISOU	214	CB	LYS A 368	3420	3345	3328	102	70	-38	A	C
ATOM	217	CG	LYS A 368	18.917	-14.709	4.899	1.00	29.26		A	C
ANISOU	217	CG	LYS A 368	3742	3825	3549	-4	-5	-10	A	C
ATOM	220	CD	LYS A 368	20.040	-15.602	4.370	1.00	32.61		A	C
ANISOU	220	CD	LYS A 368	4138	4104	4147	111	24	-9	A	C
ATOM	223	CE	LYS A 368	21.344	-15.287	5.110	1.00	35.31		A	C
ANISOU	223	CE	LYS A 368	4408	4534	4471	1	-23	8	A	C
ATOM	226	NZ	LYS A 368	22.238	-14.309	4.409	1.00	35.68		A	N
ANISOU	226	NZ	LYS A 368	4507	4521	4526	9	88	-3	A	N
ATOM	230	C	LYS A 368	16.210	-14.058	5.997	1.00	25.27		A	C
ANISOU	230	C	LYS A 368	3326	3192	3080	43	55	-57	A	C
ATOM	231	O	LYS A 368	15.570	-15.062	6.300	1.00	24.96		A	O
ANISOU	231	O	LYS A 368	3458	3127	2897	177	113	-155	A	O
ATOM	232	N	LEU A 369	16.573	-13.125	6.878	1.00	25.10		A	N
ANISOU	232	N	LEU A 369	3315	3182	3039	78	66	-53	A	N
ATOM	234	CA	LEU A 369	16.266	-13.257	8.300	1.00	25.07		A	C
ANISOU	234	CA	LEU A 369	3223	3215	3085	93	35	28	A	C
ATOM	236	CB	LEU A 369	17.406	-12.696	9.139	1.00	25.33		A	C
ANISOU	236	CB	LEU A 369	3298	3229	3097	50	60	-23	A	C
ATOM	239	CG	LEU A 369	18.724	-13.470	9.080	1.00	26.97		A	C
ANISOU	239	CG	LEU A 369	3382	3515	3350	81	26	26	A	C
ATOM	241	CD1	LEU A 369	19.769	-12.846	10.004	1.00	28.09		A	C
ANISOU	241	CD1	LEU A 369	3626	3587	3456	35	52	-51	A	C
ATOM	245	CD2	LEU A 369	18.511	-14.938	9.412	1.00	28.67		A	C
ANISOU	245	CD2	LEU A 369	3665	3660	3568	60	12	0	A	C
ATOM	249	C	LEU A 369	14.958	-12.555	8.648	1.00	24.54		A	C
ANISOU	249	C	LEU A 369	3241	3092	2990	127	46	-12	A	C
ATOM	250	O	LEU A 369	14.498	-12.610	9.779	1.00	23.69		A	O
ANISOU	250	O	LEU A 369	3083	3005	2912	274	65	66	A	O
ATOM	251	N	LEU A 370	14.371	-11.902	7.656	1.00	24.14		A	N
ANISOU	251	N	LEU A 370	3146	3093	2933	136	16	-12	A	N
ATOM	253	CA	LEU A 370	13.096	-11.200	7.797	1.00	23.76		A	C
ANISOU	253	CA	LEU A 370	3085	3033	2909	74	25	-8	A	C
ATOM	255	CB	LEU A 370	13.187	-9.807	7.157	1.00	23.77		A	C
ANISOU	255	CB	LEU A 370	3048	3055	2926	86	58	-25	A	C
ATOM	258	CG	LEU A 370	11.927	-8.942	7.067	1.00	22.97		A	C
ANISOU	258	CG	LEU A 370	3029	2940	2757	34	4	-22	A	C
ATOM	260	CD1	LEU A 370	11.524	-8.499	8.475	1.00	21.63		A	C
ANISOU	260	CD1	LEU A 370	2802	2665	2751	47	75	-70	A	C
ATOM	264	CD2	LEU A 370	12.147	-7.700	6.164	1.00	23.04		A	C
ANISOU	264	CD2	LEU A 370	3066	2926	2760	120	89	-60	A	C

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Figure 1A – 5

ATOM	268	C	LEU A 370	11.986	-11.969	7.107	1.00	23.85		A	C
ANISOU	268	C	LEU A 370	3152	2968	2941	71	-14	13	A	C
ATOM	269	O	LEU A 370	12.139	-12.367	5.943	1.00	24.72		A	O
ANISOU	269	O	LEU A 370	3366	3094	2932	51	-2	-104	A	O
ATOM	270	N	THR A 371	10.875	-12.157	7.806	1.00	22.98		A	N
ANISOU	270	N	THR A 371	3078	2849	2804	46	-33	38	A	N
ATOM	272	CA	THR A 371	9.656	-12.736	7.240	1.00	23.43		A	C
ANISOU	272	CA	THR A 371	3107	2930	2864	24	-32	27	A	C
ATOM	274	CB	THR A 371	9.225	-13.978	8.016	1.00	23.75		A	C
ANISOU	274	CB	THR A 371	3083	2989	2950	-47	-38	1	A	C
ATOM	276	OG1	THR A 371	10.188	-15.010	7.790	1.00	26.50		A	O
ANISOU	276	OG1	THR A 371	3808	3156	3104	178	56	3	A	O
ATOM	278	CG2	THR A 371	7.886	-14.548	7.516	1.00	24.49		A	C
ANISOU	278	CG2	THR A 371	3207	3026	3071	-25	-21	30	A	C
ATOM	282	C	THR A 371	8.534	-11.730	7.290	1.00	23.07		A	C
ANISOU	282	C	THR A 371	3044	2878	2843	4	-5	-18	A	C
ATOM	283	O	THR A 371	8.201	-11.202	8.359	1.00	22.03		A	O
ANISOU	283	O	THR A 371	2941	2726	2701	62	0	23	A	O
ATOM	284	N	LEU A 372	7.967	-11.447	6.124	1.00	23.05		A	N
ANISOU	284	N	LEU A 372	3077	2902	2778	14	-28	-73	A	N
ATOM	286	CA	LEU A 372	6.821	-10.564	6.010	1.00	23.79		A	C
ANISOU	286	CA	LEU A 372	3167	2982	2887	-8	-62	-49	A	C
ATOM	288	CB	LEU A 372	6.905	-9.796	4.696	1.00	24.75		A	C
ANISOU	288	CB	LEU A 372	3287	3089	3027	-33	-36	-7	A	C
ATOM	291	CG	LEU A 372	8.085	-8.847	4.584	1.00	25.08		A	C
ANISOU	291	CG	LEU A 372	3227	3157	3144	-3	8	-20	A	C
ATOM	293	CD1	LEU A 372	8.059	-8.180	3.222	1.00	27.32		A	C
ANISOU	293	CD1	LEU A 372	3631	3404	3346	-51	-28	37	A	C
ATOM	297	CD2	LEU A 372	8.050	-7.821	5.673	1.00	25.66		A	C
ANISOU	297	CD2	LEU A 372	3331	3182	3236	35	5	-5	A	C
ATOM	301	C	LEU A 372	5.576	-11.395	6.020	1.00	24.14		A	C
ANISOU	301	C	LEU A 372	3215	3022	2934	19	-38	7	A	C
ATOM	302	O	LEU A 372	5.464	-12.366	5.250	1.00	24.49		A	O
ANISOU	302	O	LEU A 372	3424	2978	2902	-68	-24	-77	A	O
ATOM	303	N	GLU A 373	4.636	-11.045	6.876	1.00	24.80		A	N
ANISOU	303	N	GLU A 373	3308	3111	3002	12	-59	-33	A	N
ATOM	305	CA	GLU A 373	3.388	-11.755	6.974	1.00	26.53		A	C
ANISOU	305	CA	GLU A 373	3451	3327	3302	-8	-37	-26	A	C
ATOM	307	CB	GLU A 373	2.997	-11.882	8.444	1.00	26.87		A	C
ANISOU	307	CB	GLU A 373	3490	3361	3356	-66	-19	-73	A	C
ATOM	310	CG	GLU A 373	4.038	-12.747	9.174	1.00	29.50		A	C
ANISOU	310	CG	GLU A 373	3832	3659	3716	15	-66	32	A	C
ATOM	313	CD	GLU A 373	3.970	-12.732	10.702	1.00	32.70		A	C
ANISOU	313	CD	GLU A 373	4348	4136	3941	70	34	35	A	C
ATOM	314	OE1	GLU A 373	3.573	-11.702	11.292	1.00	34.12		A	O
ANISOU	314	OE1	GLU A 373	4671	4133	4160	55	9	-47	A	O
ATOM	315	OE2	GLU A 373	4.340	-13.767	11.324	1.00	33.33		A	O
ANISOU	315	OE2	GLU A 373	4254	4047	4363	47	-35	13	A	O
ATOM	316	C	GLU A 373	2.325	-11.071	6.106	1.00	27.15		A	C
ANISOU	316	C	GLU A 373	3556	3408	3351	-1	-45	-31	A	C
ATOM	317	O	GLU A 373	2.560	-10.006	5.535	1.00	27.32		A	O
ANISOU	317	O	GLU A 373	3670	3415	3293	-93	-86	-34	A	O
ATOM	318	N	ASP A 374	1.180	-11.715	5.954	1.00	28.65		A	N
ANISOU	318	N	ASP A 374	3678	3576	3630	-16	-31	-11	A	N
ATOM	320	CA	ASP A 374	0.112	-11.173	5.124	1.00	30.08		A	C
ANISOU	320	CA	ASP A 374	3847	3793	3786	0	-61	2	A	C
ATOM	322	CB	ASP A 374	-0.920	-12.264	4.850	1.00	31.39		A	C
ANISOU	322	CB	ASP A 374	3927	3993	4004	-35	-66	-4	A	C
ATOM	325	CG	ASP A 374	-0.370	-13.382	3.986	1.00	35.40		A	C
ANISOU	325	CG	ASP A 374	4541	4433	4475	67	-24	-104	A	C
ATOM	326	OD1	ASP A 374	0.534	-13.117	3.142	1.00	39.57		A	O
ANISOU	326	OD1	ASP A 374	5080	5029	4923	-44	94	-33	A	O

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Figure 1A – 6

ATOM	327	OD2	ASP	A	374	-0.793	-14.560	4.084	1.00	39.52	A	O	
ANISOU	327	OD2	ASP	A	374	5129	4776	5108	-84	-54	-25	A	O
ATOM	328	C	ASP	A	374	-0.578	-9.954	5.753	1.00	29.69	A	C	
ANISOU	328	C	ASP	A	374	3778	3776	3726	0	-30	19	A	C
ATOM	329	O	ASP	A	374	-1.057	-9.073	5.045	1.00	29.69	A	O	
ANISOU	329	O	ASP	A	374	3797	3806	3675	-52	-177	74	A	O
ATOM	330	N	LYS	A	375	-0.602	-9.879	7.082	1.00	29.31	A	N	
ANISOU	330	N	LYS	A	375	3757	3729	3650	0	-48	31	A	N
ATOM	332	CA	LYS	A	375	-1.355	-8.825	7.759	1.00	28.91	A	C	
ANISOU	332	CA	LYS	A	375	3690	3665	3627	2	-48	8	A	C
ATOM	334	CB	LYS	A	375	-1.455	-9.096	9.270	1.00	28.97	A	C	
ANISOU	334	CB	LYS	A	375	3692	3650	3665	4	6	22	A	C
ATOM	337	CG	LYS	A	375	-2.227	-8.024	10.067	1.00	29.51	A	C	
ANISOU	337	CG	LYS	A	375	3817	3743	3649	14	-23	-17	A	C
ATOM	340	CD	LYS	A	375	-3.707	-7.958	9.689	1.00	30.86	A	C	
ANISOU	340	CD	LYS	A	375	3870	3845	4009	10	-12	-18	A	C
ATOM	343	CE	LYS	A	375	-4.468	-6.938	10.566	1.00	32.40	A	C	
ANISOU	343	CE	LYS	A	375	4124	4094	4090	21	42	-74	A	C
ATOM	346	NZ	LYS	A	375	-5.933	-6.873	10.266	1.00	34.42	A	N	
ANISOU	346	NZ	LYS	A	375	4290	4396	4391	30	-49	30	A	N
ATOM	350	C	LYS	A	375	-0.784	-7.426	7.481	1.00	28.46	A	C	
ANISOU	350	C	LYS	A	375	3606	3616	3592	-8	-43	18	A	C
ATOM	351	O	LYS	A	375	0.409	-7.141	7.718	1.00	28.46	A	O	
ANISOU	351	O	LYS	A	375	3659	3629	3524	-42	-76	-5	A	O
ATOM	352	N	GLU	A	376	-1.616	-6.579	6.888	1.00	28.41	A	N	
ANISOU	352	N	GLU	A	376	3587	3618	3586	-3	-36	-28	A	N
ATOM	354	CA	GLU	A	376	-1.243	-5.199	6.663	1.00	28.73	A	C	
ANISOU	354	CA	GLU	A	376	3649	3652	3614	3	-62	-23	A	C
ATOM	356	CB	GLU	A	376	-1.915	-4.656	5.409	1.00	30.02	A	C	
ANISOU	356	CB	GLU	A	376	3826	3827	3753	41	-58	29	A	C
ATOM	359	CG	AGLU	A	376	-1.222	-3.434	4.826	0.50	31.02	A	C	
ANISOU	359	CG	AGLU	A	376	3944	3929	3911	-19	-19	3	A	C
ATOM	360	CG	BGLU	A	376	-1.124	-3.565	4.724	0.50	31.42	A	C	
ANISOU	360	CG	BGLU	A	376	3970	3978	3987	-25	-19	20	A	C
ATOM	365	CD	AGLU	A	376	-1.978	-2.823	3.658	0.50	32.36	A	C	
ANISOU	365	CD	AGLU	A	376	4099	4133	4062	42	-63	15	A	C
ATOM	366	CD	BGLU	A	376	-1.471	-3.482	3.257	0.50	33.25	A	C	
ANISOU	366	CD	BGLU	A	376	4241	4282	4108	1	-54	15	A	C
ATOM	367	OE1AGLU	A	376	-2.963	-2.098	3.901	0.50	32.64	A	O		
ANISOU	367	OE1AGLU	A	376	4147	4219	4033	35	-68	4	A	O	
ATOM	368	OE1BGLU	A	376	-0.708	-4.029	2.428	0.50	34.89	A	O		
ANISOU	368	OE1BGLU	A	376	4351	4531	4375	39	11	-33	A	O	
ATOM	369	OE2AGLU	A	376	-1.580	-3.058	2.498	0.50	33.99	A	O		
ANISOU	369	OE2AGLU	A	376	4323	4407	4183	60	-11	-4	A	O	
ATOM	370	OE2BGLU	A	376	-2.526	-2.896	2.945	0.50	33.89	A	O		
ANISOU	370	OE2BGLU	A	376	4231	4379	4266	95	-22	-22	A	O	
ATOM	371	C	GLU	A	376	-1.721	-4.421	7.862	1.00	27.64	A	C	
ANISOU	371	C	GLU	A	376	3478	3498	3523	-2	-84	-34	A	C
ATOM	372	O	GLU	A	376	-2.889	-4.467	8.224	1.00	28.37	A	O	
ANISOU	372	O	GLU	A	376	3560	3588	3630	-55	-144	-152	A	O
ATOM	373	N	LEU	A	377	-0.804	-3.737	8.523	1.00	25.96	A	N	
ANISOU	373	N	LEU	A	377	3244	3256	3362	9	-71	-103	A	N
ATOM	375	CA	LEU	A	377	-1.166	-2.958	9.696	1.00	25.19	A	C	
ANISOU	375	CA	LEU	A	377	3161	3208	3200	24	-96	-37	A	C
ATOM	377	CB	LEU	A	377	0.066	-2.784	10.580	1.00	24.07	A	C	
ANISOU	377	CB	LEU	A	377	3045	2992	3107	-27	-92	-75	A	C
ATOM	380	CG	LEU	A	377	0.569	-4.095	11.180	1.00	23.12	A	C	
ANISOU	380	CG	LEU	A	377	2910	2979	2895	-30	-65	-103	A	C
ATOM	382	CD1	LEU	A	377	1.904	-3.813	11.848	1.00	21.40	A	C	
ANISOU	382	CD1	LEU	A	377	2696	2654	2781	11	-38	-49	A	C
ATOM	386	CD2	LEU	A	377	-0.410	-4.682	12.155	1.00	23.11	A	C	
ANISOU	386	CD2	LEU	A	377	2979	2862	2939	-67	-30	-132	A	C

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Figure 1A – 7

ATOM	390	C	LEU A 377	-1.694	-1.591	9.305	1.00	25.15		A	C
ANISOU	390	C	LEU A 377	3158	3172	3224	-23	-103	-41	A	C
ATOM	391	O	LEU A 377	-2.566	-1.045	9.987	1.00	23.99		A	O
ANISOU	391	O	LEU A 377	3076	2922	3117	1	-223	-107	A	O
ATOM	392	N	GLY A 378	-1.137	-1.037	8.230	1.00	26.14		A	N
ANISOU	392	N	GLY A 378	3295	3363	3271	-20	-86	-84	A	N
ATOM	394	CA	GLY A 378	-1.541	0.262	7.731	1.00	27.72		A	C
ANISOU	394	CA	GLY A 378	3497	3503	3532	19	-54	-42	A	C
ATOM	397	C	GLY A 378	-0.942	0.592	6.376	1.00	28.91		A	C
ANISOU	397	C	GLY A 378	3638	3716	3627	19	-56	-41	A	C
ATOM	398	O	GLY A 378	-0.278	-0.234	5.756	1.00	28.31		A	O
ANISOU	398	O	GLY A 378	3539	3648	3570	84	-172	-57	A	O
ATOM	399	N	SER A 379	-1.188	1.811	5.905	1.00	31.60		A	N
ANISOU	399	N	SER A 379	4029	3956	4018	60	-28	-21	A	N
ATOM	401	CA	SER A 379	-0.666	2.264	4.625	1.00	33.80		A	C
ANISOU	401	CA	SER A 379	4288	4280	4272	35	4	14	A	C
ATOM	403	CB	SER A 379	-1.526	1.711	3.503	1.00	33.96		A	C
ANISOU	403	CB	SER A 379	4332	4267	4304	51	-9	-3	A	C
ATOM	406	OG	SER A 379	-2.852	2.182	3.636	1.00	35.86		A	O
ANISOU	406	OG	SER A 379	4446	4683	4493	59	-12	23	A	O
ATOM	408	C	SER A 379	-0.643	3.788	4.536	1.00	35.35		A	C
ANISOU	408	C	SER A 379	4524	4410	4497	49	-5	21	A	C
ATOM	409	O	SER A 379	-1.275	4.478	5.342	1.00	35.41		A	O
ANISOU	409	O	SER A 379	4583	4401	4469	83	5	78	A	O
ATOM	410	N	GLY A 380	0.090	4.295	3.544	1.00	37.33		A	N
ANISOU	410	N	GLY A 380	4773	4698	4710	31	16	38	A	N
ATOM	412	CA	GLY A 380	0.204	5.727	3.306	1.00	38.31		A	C
ANISOU	412	CA	GLY A 380	4882	4802	4871	0	-6	24	A	C
ATOM	415	C	GLY A 380	0.704	5.996	1.900	1.00	39.29		A	C
ANISOU	415	C	GLY A 380	5012	4964	4951	29	-5	21	A	C
ATOM	416	O	GLY A 380	0.662	5.120	1.046	1.00	39.59		A	O
ANISOU	416	O	GLY A 380	5100	4966	4976	46	-50	38	A	O
ATOM	417	N	ASN A 381	1.174	7.217	1.662	1.00	40.44		A	N
ANISOU	417	N	ASN A 381	5143	5081	5140	3	2	25	A	N
ATOM	419	CA	ASN A 381	1.688	7.607	0.351	1.00	40.95		A	C
ANISOU	419	CA	ASN A 381	5208	5168	5180	33	22	17	A	C
ATOM	421	CB	ASN A 381	1.937	9.118	0.295	1.00	42.10		A	C
ANISOU	421	CB	ASN A 381	5372	5266	5357	5	36	20	A	C
ATOM	424	CG	ASN A 381	3.128	9.543	1.130	1.00	44.87		A	C
ANISOU	424	CG	ASN A 381	5657	5673	5716	0	-50	-48	A	C
ATOM	425	OD1	ASN A 381	3.131	9.384	2.358	1.00	48.43		A	O
ANISOU	425	OD1	ASN A 381	6250	6156	5992	22	69	34	A	O
ATOM	426	ND2	ASN A 381	4.160	10.078	0.471	1.00	47.56		A	N
ANISOU	426	ND2	ASN A 381	6041	5988	6040	-68	119	21	A	N
ATOM	429	C	ASN A 381	2.985	6.890	0.031	1.00	40.00		A	C
ANISOU	429	C	ASN A 381	5087	5061	5049	24	-1	28	A	C
ATOM	430	O	ASN A 381	3.297	6.649	-1.134	1.00	40.47		A	O
ANISOU	430	O	ASN A 381	5199	5075	5103	49	20	30	A	O
ATOM	431	N	PHE A 382	3.732	6.549	1.075	1.00	38.54		A	N
ANISOU	431	N	PHE A 382	4874	4863	4905	17	27	-13	A	N
ATOM	433	CA	PHE A 382	5.004	5.856	0.922	1.00	37.08		A	C
ANISOU	433	CA	PHE A 382	4742	4653	4693	-5	-6	10	A	C
ATOM	435	CB	PHE A 382	5.764	5.881	2.242	1.00	36.93		A	C
ANISOU	435	CB	PHE A 382	4724	4639	4669	3	22	10	A	C
ATOM	438	CG	PHE A 382	4.986	5.307	3.382	1.00	36.94		A	C
ANISOU	438	CG	PHE A 382	4733	4631	4669	-1	39	8	A	C
ATOM	439	CD1	PHE A 382	4.934	3.934	3.588	1.00	36.51		A	C
ANISOU	439	CD1	PHE A 382	4666	4575	4629	-5	20	-23	A	C
ATOM	441	CE1	PHE A 382	4.215	3.409	4.629	1.00	35.98		A	C
ANISOU	441	CE1	PHE A 382	4631	4478	4561	-3	-21	3	A	C
ATOM	443	CZ	PHE A 382	3.530	4.240	5.480	1.00	36.80		A	C
ANISOU	443	CZ	PHE A 382	4733	4610	4637	15	16	8	A	C

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## Figure 1A – 8

ATOM	445	CE2	PHE A 382	3.567	5.610	5.283	1.00	36.95		A	C
ANISOU	445	CE2	PHE A 382	4737	4608	4691	5	34	6	A	C
ATOM	447	CD2	PHE A 382	4.295	6.133	4.238	1.00	36.72		A	C
ANISOU	447	CD2	PHE A 382	4731	4558	4662	20	33	0	A	C
ATOM	449	C	PHE A 382	4.807	4.411	0.501	1.00	35.32		A	C
ANISOU	449	C	PHE A 382	4519	4452	4447	0	7	55	A	C
ATOM	450	O	PHE A 382	5.662	3.836	-0.174	1.00	35.18		A	O
ANISOU	450	O	PHE A 382	4573	4315	4477	40	0	117	A	O
ATOM	451	N	GLY A 383	3.683	3.829	0.911	1.00	33.75		A	N
ANISOU	451	N	GLY A 383	4357	4227	4236	23	-33	33	A	N
ATOM	453	CA	GLY A 383	3.400	2.427	0.632	1.00	32.46		A	C
ANISOU	453	CA	GLY A 383	4158	4117	4055	3	-3	14	A	C
ATOM	456	C	GLY A 383	2.623	1.747	1.750	1.00	30.90		A	C
ANISOU	456	C	GLY A 383	3992	3873	3875	67	-44	45	A	C
ATOM	457	O	GLY A 383	1.545	2.209	2.130	1.00	31.35		A	O
ANISOU	457	O	GLY A 383	4087	3976	3847	75	-25	132	A	O
ATOM	458	N	THR A 384	3.145	0.646	2.302	1.00	28.79		A	N
ANISOU	458	N	THR A 384	3698	3670	3569	61	-19	28	A	N
ATOM	460	CA	THR A 384	2.388	-0.079	3.313	1.00	27.47		A	C
ANISOU	460	CA	THR A 384	3539	3478	3417	69	-73	16	A	C
ATOM	462	CB	THR A 384	1.914	-1.423	2.747	1.00	28.10		A	C
ANISOU	462	CB	THR A 384	3596	3599	3478	3	-67	9	A	C
ATOM	464	OG1	THR A 384	3.055	-2.187	2.333	1.00	29.24		A	O
ANISOU	464	OG1	THR A 384	3900	3575	3632	56	-70	-8	A	O
ATOM	466	CG2	THR A 384	1.086	-1.203	1.465	1.00	28.51		A	C
ANISOU	466	CG2	THR A 384	3696	3636	3501	-13	-104	0	A	C
ATOM	470	C	THR A 384	3.220	-0.370	4.557	1.00	25.43		A	C
ANISOU	470	C	THR A 384	3290	3210	3160	62	-26	47	A	C
ATOM	471	O	THR A 384	4.423	-0.192	4.543	1.00	24.13		A	O
ANISOU	471	O	THR A 384	3221	3065	2881	208	-144	100	A	O
ATOM	472	N	VAL A 385	2.535	-0.743	5.633	1.00	23.59		A	N
ANISOU	472	N	VAL A 385	3066	2941	2954	116	-69	17	A	N
ATOM	474	CA	VAL A 385	3.192	-1.272	6.823	1.00	22.63		A	C
ANISOU	474	CA	VAL A 385	2947	2871	2779	50	-25	-49	A	C
ATOM	476	CB	VAL A 385	3.009	-0.350	8.061	1.00	22.43		A	C
ANISOU	476	CB	VAL A 385	2908	2860	2751	53	-16	-50	A	C
ATOM	478	CG1	VAL A 385	3.716	-0.907	9.262	1.00	21.76		A	C
ANISOU	478	CG1	VAL A 385	2791	2716	2759	56	54	-87	A	C
ATOM	482	CG2	VAL A 385	3.522	1.014	7.727	1.00	23.07		A	C
ANISOU	482	CG2	VAL A 385	3061	2915	2787	-24	-78	-103	A	C
ATOM	486	C	VAL A 385	2.632	-2.661	7.097	1.00	21.57		A	C
ANISOU	486	C	VAL A 385	2830	2755	2610	52	-44	-59	A	C
ATOM	487	O	VAL A 385	1.425	-2.826	7.314	1.00	21.06		A	O
ANISOU	487	O	VAL A 385	2772	2662	2567	156	-156	-25	A	O
ATOM	488	N	LYS A 386	3.511	-3.659	7.097	1.00	21.67		A	N
ANISOU	488	N	LYS A 386	2867	2767	2600	29	-21	-21	A	N
ATOM	490	CA	LYS A 386	3.101	-5.047	7.297	1.00	21.49		A	C
ANISOU	490	CA	LYS A 386	2841	2721	2603	42	-18	-7	A	C
ATOM	492	CB	LYS A 386	3.579	-5.915	6.119	1.00	22.52		A	C
ANISOU	492	CB	LYS A 386	2976	2764	2815	14	25	-33	A	C
ATOM	495	CG	LYS A 386	2.862	-5.616	4.815	1.00	25.83		A	C
ANISOU	495	CG	LYS A 386	3338	3336	3140	11	-85	72	A	C
ATOM	498	CD	LYS A 386	3.333	-6.534	3.669	1.00	30.90		A	C
ANISOU	498	CD	LYS A 386	3956	3973	3810	76	31	-130	A	C
ATOM	501	CE	LYS A 386	2.380	-7.705	3.426	1.00	34.41		A	C
ANISOU	501	CE	LYS A 386	4337	4328	4409	-71	4	-9	A	C
ATOM	504	NZ	LYS A 386	3.036	-8.851	2.716	1.00	37.23		A	N
ANISOU	504	NZ	LYS A 386	4765	4700	4679	41	5	-115	A	N
ATOM	508	C	LYS A 386	3.707	-5.639	8.549	1.00	20.53		A	C
ANISOU	508	C	LYS A 386	2706	2595	2497	46	19	-25	A	C
ATOM	509	O	LYS A 386	4.769	-5.233	8.973	1.00	19.95		A	O
ANISOU	509	O	LYS A 386	2807	2516	2254	92	-23	-29	A	O



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## Figure 1A - 9

ATOM	510	N	LYS	A	387	3.014	-6.620	9.102	1.00	20.61	A	N	
ANISOU	510	N	LYS	A	387	2751	2547	2533	29	-54	-50	A	N
ATOM	512	CA	LYS	A	387	3.535	-7.408	10.205	1.00	20.28	A	C	
ANISOU	512	CA	LYS	A	387	2702	2554	2447	10	-44	-17	A	C
ATOM	514	CB	LYS	A	387	2.456	-8.341	10.751	1.00	21.91	A	C	
ANISOU	514	CB	LYS	A	387	2862	2766	2695	-35	-29	51	A	C
ATOM	517	CG	LYS	A	387	1.534	-7.767	11.711	1.00	23.35	A	C	
ANISOU	517	CG	LYS	A	387	3023	2925	2922	19	10	0	A	C
ATOM	520	CD	LYS	A	387	0.619	-8.810	12.393	1.00	23.54	A	C	
ANISOU	520	CD	LYS	A	387	2986	3003	2954	-137	-34	-83	A	C
ATOM	523	CE	LYS	A	387	1.371	-9.734	13.324	1.00	25.61	A	C	
ANISOU	523	CE	LYS	A	387	3339	3179	3211	-22	54	15	A	C
ATOM	526	NZ	LYS	A	387	0.412	-10.547	14.177	1.00	25.22	A	N	
ANISOU	526	NZ	LYS	A	387	3406	3178	2998	-81	26	56	A	N
ATOM	530	C	LYS	A	387	4.617	-8.323	9.692	1.00	20.12	A	C	
ANISOU	530	C	LYS	A	387	2678	2515	2448	16	-57	31	A	C
ATOM	531	O	LYS	A	387	4.585	-8.787	8.550	1.00	20.85	A	O	
ANISOU	531	O	LYS	A	387	2877	2582	2463	32	-92	61	A	O
ATOM	532	N	GLY	A	388	5.578	-8.610	10.537	1.00	19.87	A	N	
ANISOU	532	N	GLY	A	388	2582	2576	2390	42	-42	-15	A	N
ATOM	534	CA	GLY	A	388	6.577	-9.602	10.211	1.00	19.53	A	C	
ANISOU	534	CA	GLY	A	388	2550	2454	2417	32	-45	-23	A	C
ATOM	537	C	GLY	A	388	7.367	-10.004	11.443	1.00	19.52	A	C	
ANISOU	537	C	GLY	A	388	2520	2500	2396	31	-24	-32	A	C
ATOM	538	O	GLY	A	388	7.019	-9.641	12.567	1.00	19.06	A	O	
ANISOU	538	O	GLY	A	388	2579	2326	2335	-15	17	-117	A	O
ATOM	539	N	TYR	A	389	8.422	-10.775	11.232	1.00	18.42	A	N	
ANISOU	539	N	TYR	A	389	2478	2261	2259	12	-30	-139	A	N
ATOM	541	CA	TYR	A	389	9.311	-11.093	12.317	1.00	18.83	A	C	
ANISOU	541	CA	TYR	A	389	2461	2339	2351	21	9	-25	A	C
ATOM	543	CB	TYR	A	389	8.923	-12.399	13.010	1.00	19.50	A	C	
ANISOU	543	CB	TYR	A	389	2484	2535	2387	-26	73	-54	A	C
ATOM	546	CG	TYR	A	389	9.081	-13.639	12.197	1.00	20.52	A	C	
ANISOU	546	CG	TYR	A	389	2528	2636	2629	-20	14	70	A	C
ATOM	547	CD1	TYR	A	389	10.324	-14.215	12.046	1.00	22.45	A	C	
ANISOU	547	CD1	TYR	A	389	2876	2830	2823	47	-27	-77	A	C
ATOM	549	CE1	TYR	A	389	10.505	-15.366	11.319	1.00	22.57	A	C	
ANISOU	549	CE1	TYR	A	389	2731	2939	2903	98	-58	-69	A	C
ATOM	551	CZ	TYR	A	389	9.404	-15.984	10.722	1.00	21.58	A	C	
ANISOU	551	CZ	TYR	A	389	2973	2616	2609	-3	19	-179	A	C
ATOM	552	OH	TYR	A	389	9.621	-17.155	9.983	1.00	24.39	A	O	
ANISOU	552	OH	TYR	A	389	3282	2908	3076	-101	262	-55	A	O
ATOM	554	CE2	TYR	A	389	8.139	-15.412	10.841	1.00	22.65	A	C	
ANISOU	554	CE2	TYR	A	389	2940	2970	2693	-159	58	-27	A	C
ATOM	556	CD2	TYR	A	389	7.990	-14.239	11.590	1.00	22.98	A	C	
ANISOU	556	CD2	TYR	A	389	3099	2813	2820	-107	44	-9	A	C
ATOM	558	C	TYR	A	389	10.711	-11.122	11.800	1.00	18.66	A	C	
ANISOU	558	C	TYR	A	389	2454	2322	2313	0	24	-45	A	C
ATOM	559	O	TYR	A	389	10.937	-11.326	10.595	1.00	19.97	A	O	
ANISOU	559	O	TYR	A	389	2729	2512	2347	-105	32	-5	A	O
ATOM	560	N	TYR	A	390	11.652	-10.901	12.700	1.00	18.53	A	N	
ANISOU	560	N	TYR	A	390	2490	2314	2235	7	33	-57	A	N
ATOM	562	CA	TYR	A	390	13.052	-10.842	12.338	1.00	19.45	A	C	
ANISOU	562	CA	TYR	A	390	2497	2508	2386	46	14	-20	A	C
ATOM	564	CB	TYR	A	390	13.587	-9.409	12.368	1.00	19.00	A	C	
ANISOU	564	CB	TYR	A	390	2403	2523	2291	0	0	-22	A	C
ATOM	567	CG	TYR	A	390	14.965	-9.285	11.714	1.00	19.64	A	C	
ANISOU	567	CG	TYR	A	390	2493	2609	2360	-25	103	-37	A	C
ATOM	568	CD1	TYR	A	390	15.109	-9.301	10.332	1.00	21.12	A	C	
ANISOU	568	CD1	TYR	A	390	2739	2816	2469	-49	-15	-9	A	C
ATOM	570	CE1	TYR	A	390	16.350	-9.187	9.746	1.00	21.70	A	C	
ANISOU	570	CE1	TYR	A	390	2797	2906	2542	41	51	-181	A	C

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Figure 1A – 10

ATOM	572	CZ	TYR	A	390	17.497	-9.107	10.519	1.00	22.51		A	C
ANISOU	572	CZ	TYR	A	390	2833	3067	2652	-1	20	-25	A	C
ATOM	573	OH	TYR	A	390	18.756	-9.006	9.929	1.00	23.31		A	O
ANISOU	573	OH	TYR	A	390	3041	3150	2662	80	118	-120	A	O
ATOM	575	CE2	TYR	A	390	17.382	-9.112	11.894	1.00	23.03		A	C
ANISOU	575	CE2	TYR	A	390	2978	3042	2727	-33	64	-43	A	C
ATOM	577	CD2	TYR	A	390	16.105	-9.198	12.472	1.00	21.52		A	C
ANISOU	577	CD2	TYR	A	390	2748	2960	2467	41	-16	17	A	C
ATOM	579	C	TYR	A	390	13.869	-11.738	13.246	1.00	20.22		A	C
ANISOU	579	C	TYR	A	390	2628	2608	2444	47	19	31	A	C
ATOM	580	O	TYR	A	390	13.761	-11.666	14.467	1.00	18.74		A	O
ANISOU	580	O	TYR	A	390	2395	2500	2222	-62	120	95	A	O
ATOM	581	N	GLN	A	391	14.722	-12.574	12.655	1.00	21.83		A	N
ANISOU	581	N	GLN	A	391	2829	2839	2624	103	78	1	A	N
ATOM	583	CA	GLN	A	391	15.525	-13.485	13.482	1.00	23.36		A	C
ANISOU	583	CA	GLN	A	391	2983	3020	2871	99	31	3	A	C
ATOM	585	CB	GLN	A	391	15.947	-14.704	12.673	1.00	23.78		A	C
ANISOU	585	CB	GLN	A	391	3107	3024	2905	116	12	13	A	C
ATOM	588	CG	AGLN	A	391	16.676	-15.931	13.376	0.60	23.48		A	C
ANISOU	588	CG	AGLN	A	391	2898	3101	2920	91	20	-6	A	C
ATOM	589	CG	BGLN	A	391	15.232	-15.986	13.065	0.40	26.06		A	C
ANISOU	589	CG	BGLN	A	391	3278	3294	3328	-12	49	-43	A	C
ATOM	594	CD	AGLN	A	391	16.099	-16.513	14.654	0.60	22.52		A	C
ANISOU	594	CD	AGLN	A	391	2921	2857	2778	-18	-13	-93	A	C
ATOM	595	CD	BGLN	A	391	14.547	-16.665	11.868	0.40	27.58		A	C
ANISOU	595	CD	BGLN	A	391	3464	3617	3398	1	-50	-23	A	C
ATOM	596	OE1AGLN	A	391		15.366	-17.549	14.619	0.60	20.95		A	O
ANISOU	596	OE1AGLN	A	391		2491	3077	2389	-88	199	-164	A	O
ATOM	597	OE1BGLN	A	391		13.549	-17.372	12.040	0.40	28.64		A	O
ANISOU	597	OE1BGLN	A	391		3693	3529	3659	-25	-11	-18	A	O
ATOM	598	NE2AGLN	A	391		16.516	-15.935	15.807	0.60	18.15		A	N
ANISOU	598	NE2AGLN	A	391		2289	2328	2276	136	-37	68	A	N
ATOM	599	NE2BGLN	A	391		15.083	-16.453	10.663	0.40	28.06		A	N
ANISOU	599	NE2BGLN	A	391		3582	3512	3568	12	53	61	A	N
ATOM	604	C	GLN	A	391	16.753	-12.749	14.000	1.00	24.01		A	C
ANISOU	604	C	GLN	A	391	3016	3098	3007	31	48	0	A	C
ATOM	605	O	GLN	A	391	17.621	-12.385	13.237	1.00	25.54		A	O
ANISOU	605	O	GLN	A	391	3197	3506	2999	63	67	0	A	O
ATOM	606	N	MET	A	392	16.808	-12.498	15.302	1.00	24.76		A	N
ANISOU	606	N	MET	A	392	3119	3260	3028	19	55	13	A	N
ATOM	608	CA	MET	A	392	17.932	-11.826	15.930	1.00	25.39		A	C
ANISOU	608	CA	MET	A	392	3183	3287	3173	-27	73	36	A	C
ATOM	610	CB	MET	A	392	17.463	-11.046	17.188	1.00	25.63		A	C
ANISOU	610	CB	MET	A	392	3261	3274	3201	-95	27	19	A	C
ATOM	613	CG	MET	A	392	16.236	-10.144	17.009	1.00	26.84		A	C
ANISOU	613	CG	MET	A	392	3547	3360	3289	-56	23	19	A	C
ATOM	616	SD	MET	A	392	16.610	-8.592	16.133	1.00	30.68		A	S
ANISOU	616	SD	MET	A	392	4543	3645	3467	-288	82	90	A	S
ATOM	617	CE	MET	A	392	17.186	-7.583	17.455	1.00	30.77		A	C
ANISOU	617	CE	MET	A	392	4076	3820	3795	-39	42	-47	A	C
ATOM	621	C	MET	A	392	18.998	-12.880	16.294	1.00	25.71		A	C
ANISOU	621	C	MET	A	392	3222	3348	3198	-14	100	36	A	C
ATOM	622	O	MET	A	392	18.903	-14.030	15.872	1.00	24.92		A	O
ANISOU	622	O	MET	A	392	2880	3468	3119	46	139	79	A	O
ATOM	623	N	LYS	A	393	19.947	-12.471	17.138	1.00	27.71		A	N
ANISOU	623	N	LYS	A	393	3392	3685	3450	-16	81	77	A	N
ATOM	625	CA	LYS	A	393	21.079	-13.274	17.633	1.00	28.99		A	C
ANISOU	625	CA	LYS	A	393	3624	3746	3642	36	51	35	A	C
ATOM	627	CB	LYS	A	393	21.719	-12.508	18.816	1.00	30.45		A	C
ANISOU	627	CB	LYS	A	393	3851	3887	3827	-11	-24	14	A	C
ATOM	630	CG	LYS	A	393	23.222	-12.347	18.807	1.00	34.82		A	C
ANISOU	630	CG	LYS	A	393	4277	4495	4457	-2	57	56	A	C

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Figure 1A – 11

ATOM	633	CD	LYS	A	393	23.727	-11.364	19.906	1.00	38.33		A	C
ANISOU	633	CD	LYS	A	393	4894	4822	4847	-37	-37	-64	A	C
ATOM	636	CE	LYS	A	393	22.729	-11.132	21.066	1.00	40.36		A	C
ANISOU	636	CE	LYS	A	393	5070	5156	5107	-40	33	-8	A	C
ATOM	639	NZ	LYS	A	393	22.785	-9.748	21.630	1.00	42.97		A	N
ANISOU	639	NZ	LYS	A	393	5534	5281	5511	55	11	-45	A	N
ATOM	643	C	LYS	A	393	20.607	-14.633	18.150	1.00	27.65		A	C
ANISOU	643	C	LYS	A	393	3435	3608	3464	46	42	0	A	C
ATOM	644	O	LYS	A	393	21.138	-15.699	17.818	1.00	27.67		A	O
ANISOU	644	O	LYS	A	393	3301	3763	3447	98	85	-28	A	O
ATOM	645	N	LYS	A	394	19.592	-14.574	19.003	1.00	24.84		A	N
ANISOU	645	N	LYS	A	394	3038	3255	3145	72	-1	-1	A	N
ATOM	647	CA	LYS	A	394	19.010	-15.744	19.592	1.00	23.15		A	C
ANISOU	647	CA	LYS	A	394	2765	3073	2956	38	-15	-20	A	C
ATOM	649	CB	LYS	A	394	19.395	-15.787	21.068	1.00	22.45		A	C
ANISOU	649	CB	LYS	A	394	2700	2965	2862	50	21	-5	A	C
ATOM	652	CG	LYS	A	394	18.752	-16.924	21.840	1.00	22.82		A	C
ANISOU	652	CG	LYS	A	394	2832	2905	2932	-51	-46	34	A	C
ATOM	655	CD	LYS	A	394	19.023	-18.281	21.266	1.00	22.02		A	C
ANISOU	655	CD	LYS	A	394	2537	2986	2841	83	54	8	A	C
ATOM	658	CE	LYS	A	394	18.732	-19.370	22.262	1.00	21.04		A	C
ANISOU	658	CE	LYS	A	394	2546	2705	2742	98	-39	-141	A	C
ATOM	661	NZ	LYS	A	394	19.850	-19.545	23.198	1.00	18.99		A	N
ANISOU	661	NZ	LYS	A	394	2331	2450	2431	21	8	-131	A	N
ATOM	665	C	LYS	A	394	17.472	-15.720	19.426	1.00	21.22		A	C
ANISOU	665	C	LYS	A	394	2572	2781	2707	-1	31	-12	A	C
ATOM	666	O	LYS	A	394	16.903	-16.613	18.828	1.00	21.83		A	O
ANISOU	666	O	LYS	A	394	2335	3085	2874	28	46	-41	A	O
ATOM	667	N	VAL	A	395	16.814	-14.697	19.943	1.00	20.14		A	N
ANISOU	667	N	VAL	A	395	2416	2707	2529	-19	-63	61	A	N
ATOM	669	CA	VAL	A	395	15.365	-14.655	19.878	1.00	19.74		A	C
ANISOU	669	CA	VAL	A	395	2439	2566	2492	10	23	27	A	C
ATOM	671	CB	VAL	A	395	14.780	-13.762	20.998	1.00	19.99		A	C
ANISOU	671	CB	VAL	A	395	2447	2651	2496	-3	-40	6	A	C
ATOM	673	CG1	VAL	A	395	15.301	-14.222	22.363	1.00	20.54		A	C
ANISOU	673	CG1	VAL	A	395	2591	2626	2586	-35	76	47	A	C
ATOM	677	CG2	VAL	A	395	15.081	-12.290	20.753	1.00	20.68		A	C
ANISOU	677	CG2	VAL	A	395	2605	2777	2474	-29	4	-82	A	C
ATOM	681	C	VAL	A	395	14.867	-14.159	18.526	1.00	19.27		A	C
ANISOU	681	C	VAL	A	395	2352	2513	2454	8	-12	-21	A	C
ATOM	682	O	VAL	A	395	15.620	-13.654	17.701	1.00	19.18		A	O
ANISOU	682	O	VAL	A	395	2270	2635	2380	33	-59	14	A	O
ATOM	683	N	VAL	A	396	13.583	-14.352	18.287	1.00	18.67		A	N
ANISOU	683	N	VAL	A	396	2281	2395	2416	-22	15	4	A	N
ATOM	685	CA	VAL	A	396	12.913	-13.724	17.164	1.00	18.40		A	C
ANISOU	685	CA	VAL	A	396	2346	2346	2296	-45	48	25	A	C
ATOM	687	CB	VAL	A	396	11.929	-14.706	16.518	1.00	18.53		A	C
ANISOU	687	CB	VAL	A	396	2322	2347	2370	-31	14	-12	A	C
ATOM	689	CG1	VAL	A	396	10.890	-14.009	15.691	1.00	20.09		A	C
ANISOU	689	CG1	VAL	A	396	2598	2529	2505	-43	-69	-29	A	C
ATOM	693	CG2	VAL	A	396	12.696	-15.699	15.675	1.00	19.72		A	C
ANISOU	693	CG2	VAL	A	396	2569	2540	2381	-53	134	0	A	C
ATOM	697	C	VAL	A	396	12.196	-12.484	17.675	1.00	18.04		A	C
ANISOU	697	C	VAL	A	396	2299	2283	2270	-18	11	79	A	C
ATOM	698	O	VAL	A	396	11.626	-12.472	18.780	1.00	17.68		A	O
ANISOU	698	O	VAL	A	396	2392	2126	2200	59	7	169	A	O
ATOM	699	N	LYS	A	397	12.246	-11.407	16.889	1.00	17.02		A	N
ANISOU	699	N	LYS	A	397	2184	2109	2172	-57	34	79	A	N
ATOM	701	CA	LYS	A	397	11.587	-10.173	17.283	1.00	17.12		A	C
ANISOU	701	CA	LYS	A	397	2147	2176	2180	-25	32	-9	A	C
ATOM	703	CB	LYS	A	397	12.605	-9.020	17.221	1.00	17.90		A	C
ANISOU	703	CB	LYS	A	397	2278	2233	2288	-33	46	-46	A	C

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Figure 1A – 12

ATOM	706	CG	LYS A 397	12.076	-7.611	17.367	1.00	18.88		A	C
ANISOU	706	CG	LYS A 397	2425	2255	2491	-88	-107	-52	A	C
ATOM	709	CD	LYS A 397	11.614	-7.347	18.784	1.00	21.72		A	C
ANISOU	709	CD	LYS A 397	2761	2750	2738	-25	83	2	A	C
ATOM	712	CE	LYS A 397	11.478	-5.840	19.030	1.00	22.96		A	C
ANISOU	712	CE	LYS A 397	3031	2778	2913	-77	34	-65	A	C
ATOM	715	NZ	LYS A 397	10.826	-5.470	20.312	1.00	23.58		A	N
ANISOU	715	NZ	LYS A 397	3025	2913	3021	-123	62	1	A	N
ATOM	719	C	LYS A 397	10.434	-9.896	16.343	1.00	16.91		A	C
ANISOU	719	C	LYS A 397	2181	2129	2114	7	23	32	A	C
ATOM	720	O	LYS A 397	10.610	-9.905	15.098	1.00	17.45		A	O
ANISOU	720	O	LYS A 397	2192	2313	2123	34	-33	-85	A	O
ATOM	721	N	THR A 398	9.241	-9.673	16.895	1.00	16.15		A	N
ANISOU	721	N	THR A 398	2163	1965	2005	-99	-18	33	A	N
ATOM	723	CA	THR A 398	8.141	-9.267	16.051	1.00	16.74		A	C
ANISOU	723	CA	THR A 398	2185	2058	2117	-46	-35	17	A	C
ATOM	725	CB	THR A 398	6.806	-9.386	16.751	1.00	17.39		A	C
ANISOU	725	CB	THR A 398	2250	2149	2207	-71	-27	-51	A	C
ATOM	727	OG1	THR A 398	6.768	-8.568	17.918	1.00	18.53		A	O
ANISOU	727	OG1	THR A 398	2462	2448	2130	-53	-20	8	A	O
ATOM	729	CG2	THR A 398	6.605	-10.803	17.253	1.00	19.59		A	C
ANISOU	729	CG2	THR A 398	2500	2395	2544	-92	17	60	A	C
ATOM	733	C	THR A 398	8.401	-7.839	15.583	1.00	16.71		A	C
ANISOU	733	C	THR A 398	2224	2054	2069	-69	-48	-1	A	C
ATOM	734	O	THR A 398	8.901	-6.991	16.336	1.00	16.76		A	O
ANISOU	734	O	THR A 398	2332	2105	1930	-50	7	26	A	O
ATOM	735	N	VAL A 399	8.048	-7.583	14.327	1.00	16.70		A	N
ANISOU	735	N	VAL A 399	2278	2003	2063	7	16	62	A	N
ATOM	737	CA	VAL A 399	8.318	-6.290	13.742	1.00	16.67		A	C
ANISOU	737	CA	VAL A 399	2220	2018	2093	-16	9	13	A	C
ATOM	739	CB	VAL A 399	9.609	-6.314	12.897	1.00	16.56		A	C
ANISOU	739	CB	VAL A 399	2252	1947	2089	16	-13	70	A	C
ATOM	741	CG1	VAL A 399	10.838	-6.581	13.763	1.00	16.05		A	C
ANISOU	741	CG1	VAL A 399	1925	2089	2083	45	100	-48	A	C
ATOM	745	CG2	VAL A 399	9.504	-7.308	11.792	1.00	17.60		A	C
ANISOU	745	CG2	VAL A 399	2329	2165	2190	-42	85	-9	A	C
ATOM	749	C	VAL A 399	7.189	-5.759	12.858	1.00	17.28		A	C
ANISOU	749	C	VAL A 399	2295	2082	2187	-24	-22	36	A	C
ATOM	750	O	VAL A 399	6.372	-6.499	12.285	1.00	18.04		A	O
ANISOU	750	O	VAL A 399	2440	2146	2268	-56	-113	96	A	O
ATOM	751	N	ALA A 400	7.160	-4.436	12.766	1.00	17.41		A	N
ANISOU	751	N	ALA A 400	2362	2022	2228	35	-14	-39	A	N
ATOM	753	CA	ALA A 400	6.325	-3.760	11.800	1.00	17.54		A	C
ANISOU	753	CA	ALA A 400	2270	2135	2257	4	-8	-2	A	C
ATOM	755	CB	ALA A 400	5.562	-2.650	12.475	1.00	17.55		A	C
ANISOU	755	CB	ALA A 400	2274	2172	2222	71	16	5	A	C
ATOM	759	C	ALA A 400	7.258	-3.212	10.735	1.00	18.59		A	C
ANISOU	759	C	ALA A 400	2460	2274	2327	44	-2	7	A	C
ATOM	760	O	ALA A 400	8.266	-2.589	11.061	1.00	18.33		A	O
ANISOU	760	O	ALA A 400	2434	2305	2226	-19	23	81	A	O
ATOM	761	N	VAL A 401	6.944	-3.475	9.466	1.00	19.43		A	N
ANISOU	761	N	VAL A 401	2537	2447	2400	20	15	-27	A	N
ATOM	763	CA	VAL A 401	7.845	-3.108	8.389	1.00	19.79		A	C
ANISOU	763	CA	VAL A 401	2639	2453	2424	49	-4	15	A	C
ATOM	765	CB	VAL A 401	8.281	-4.358	7.614	1.00	19.84		A	C
ANISOU	765	CB	VAL A 401	2654	2469	2414	54	27	-22	A	C
ATOM	767	CG1	VAL A 401	9.332	-3.996	6.601	1.00	20.47		A	C
ANISOU	767	CG1	VAL A 401	2629	2515	2631	88	27	-15	A	C
ATOM	771	CG2	VAL A 401	8.787	-5.451	8.591	1.00	20.43		A	C
ANISOU	771	CG2	VAL A 401	2667	2563	2532	19	36	30	A	C
ATOM	775	C	VAL A 401	7.218	-2.132	7.426	1.00	19.94		A	C
ANISOU	775	C	VAL A 401	2650	2533	2392	57	-9	27	A	C

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Figure 1A – 13

ATOM	776	O	VAL	A	401	6.186	-2.434	6.818	1.00	18.74		A	O
ANISOU	776	O	VAL	A	401	2756	2348	2014	113	-48	61	A	O
ATOM	777	N	LYS	A	402	7.824	-0.959	7.339	1.00	21.49		A	N
ANISOU	777	N	LYS	A	402	2906	2733	2523	21	-4	31	A	N
ATOM	779	CA	LYS	A	402	7.397	0.066	6.383	1.00	22.99		A	C
ANISOU	779	CA	LYS	A	402	3028	2918	2786	62	2	51	A	C
ATOM	781	CB	LYS	A	402	7.866	1.436	6.831	1.00	23.88		A	C
ANISOU	781	CB	LYS	A	402	3152	2986	2935	4	-18	96	A	C
ATOM	784	CG	LYS	A	402	7.359	2.581	5.967	1.00	25.78		A	C
ANISOU	784	CG	LYS	A	402	3460	3169	3164	64	-37	98	A	C
ATOM	787	CD	LYS	A	402	7.509	3.879	6.732	1.00	27.41		A	C
ANISOU	787	CD	LYS	A	402	3537	3389	3488	-47	-74	-38	A	C
ATOM	790	CE	LYS	A	402	7.141	5.066	5.920	1.00	29.80		A	C
ANISOU	790	CE	LYS	A	402	3855	3703	3763	-44	-23	10	A	C
ATOM	793	NZ	LYS	A	402	7.453	6.270	6.700	1.00	29.91		A	N
ANISOU	793	NZ	LYS	A	402	3842	3688	3831	-5	46	-105	A	N
ATOM	797	C	LYS	A	402	8.043	-0.296	5.067	1.00	23.72		A	C
ANISOU	797	C	LYS	A	402	3102	3017	2890	27	52	57	A	C
ATOM	798	O	LYS	A	402	9.269	-0.324	4.974	1.00	24.28		A	O
ANISOU	798	O	LYS	A	402	3248	3291	2687	41	182	198	A	O
ATOM	799	N	ILE	A	403	7.219	-0.588	4.075	1.00	25.19		A	N
ANISOU	799	N	ILE	A	403	3303	3194	3074	40	47	44	A	N
ATOM	801	CA	ILE	A	403	7.703	-0.994	2.755	1.00	26.13		A	C
ANISOU	801	CA	ILE	A	403	3417	3328	3183	36	13	36	A	C
ATOM	803	CB	ILE	A	403	7.073	-2.330	2.361	1.00	26.45		A	C
ANISOU	803	CB	ILE	A	403	3455	3345	3247	40	12	19	A	C
ATOM	805	CG1	ILE	A	403	7.373	-3.411	3.397	1.00	26.67		A	C
ANISOU	805	CG1	ILE	A	403	3491	3469	3173	30	-52	-2	A	C
ATOM	808	CD1	ILE	A	403	6.389	-4.530	3.316	1.00	28.98		A	C
ANISOU	808	CD1	ILE	A	403	3741	3718	3551	-50	44	31	A	C
ATOM	812	CG2	ILE	A	403	7.554	-2.789	0.978	1.00	27.44		A	C
ANISOU	812	CG2	ILE	A	403	3542	3556	3326	10	13	-29	A	C
ATOM	816	C	ILE	A	403	7.328	0.073	1.731	1.00	27.34		A	C
ANISOU	816	C	ILE	A	403	3590	3443	3355	62	-7	27	A	C
ATOM	817	O	ILE	A	403	6.184	0.450	1.614	1.00	27.60		A	O
ANISOU	817	O	ILE	A	403	3738	3468	3280	66	-22	174	A	O
ATOM	818	N	LEU	A	404	8.305	0.508	0.972	1.00	28.90		A	N
ANISOU	818	N	LEU	A	404	3810	3625	3546	2	3	34	A	N
ATOM	820	CA	LEU	A	404	8.060	1.527	-0.038	1.00	31.22		A	C
ANISOU	820	CA	LEU	A	404	4025	3907	3929	22	-14	62	A	C
ATOM	822	CB	LEU	A	404	9.380	2.134	-0.473	1.00	31.54		A	C
ANISOU	822	CB	LEU	A	404	4058	3959	3967	3	6	27	A	C
ATOM	825	CG	LEU	A	404	10.068	3.014	0.562	1.00	32.21		A	C
ANISOU	825	CG	LEU	A	404	4136	4034	4065	6	-38	12	A	C
ATOM	827	CD1	LEU	A	404	11.244	3.720	-0.089	1.00	33.07		A	C
ANISOU	827	CD1	LEU	A	404	4248	4152	4164	10	66	-26	A	C
ATOM	831	CD2	LEU	A	404	9.063	4.020	1.150	1.00	33.02		A	C
ANISOU	831	CD2	LEU	A	404	4169	4176	4200	14	5	-28	A	C
ATOM	835	C	LEU	A	404	7.357	0.901	-1.231	1.00	32.90		A	C
ANISOU	835	C	LEU	A	404	4246	4179	4073	-12	-11	14	A	C
ATOM	836	O	LEU	A	404	7.560	-0.262	-1.555	1.00	33.21		A	O
ANISOU	836	O	LEU	A	404	4287	4229	4100	2	-43	56	A	O
ATOM	837	N	LYS	A	405	6.506	1.667	-1.882	1.00	35.30		A	N
ANISOU	837	N	LYS	A	405	4502	4436	4471	21	-8	53	A	N
ATOM	839	CA	LYS	A	405	5.819	1.160	-3.058	1.00	37.77		A	C
ANISOU	839	CA	LYS	A	405	4825	4782	4743	-12	-19	0	A	C
ATOM	841	CB	LYS	A	405	4.590	2.011	-3.318	1.00	39.03		A	C
ANISOU	841	CB	LYS	A	405	4950	4976	4904	7	-28	-6	A	C
ATOM	844	CG	ALYS	A	405	4.849	3.433	-3.746	1.00	41.29		A	C
ANISOU	844	CG	ALYS	A	405	5320	5141	5225	9	1	30	A	C
ATOM	845	CG	BLYS	A	405	5.034	3.473	-3.443	1.00	40.93		A	C
ANISOU	845	CG	BLYS	A	405	5272	5114	5164	0	-19	29	A	C

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Figure 1A – 14

ATOM	850	CD	ALYS	A	405	3.518	4.233	-4.040	0.50	42.05		A	C
ANISOU	850	CD	ALYS	A	405	5301	5325	5352	17	-25	4	A	C
ATOM	851	CD	BLYS	A	405	3.847	4.482	-3.441	0.50	41.64		A	C
ANISOU	851	CD	BLYS	A	405	5260	5270	5289	31	0	4	A	C
ATOM	856	CE	ALYS	A	405	2.350	3.915	-3.098	0.50	42.51		A	C
ANISOU	856	CE	ALYS	A	405	5394	5384	5374	-4	-1	14	A	C
ATOM	857	CE	BLYS	A	405	4.162	5.661	-4.376	0.50	41.95		A	C
ANISOU	857	CE	BLYS	A	405	5318	5297	5324	-5	-1	16	A	C
ATOM	862	NZ	ALYS	A	405	1.183	4.824	-3.331	0.50	42.94		A	N
ANISOU	862	NZ	ALYS	A	405	5419	5437	5456	18	3	-7	A	N
ATOM	863	NZ	BLYS	A	405	3.610	6.958	-3.905	0.50	42.23		A	N
ANISOU	863	NZ	BLYS	A	405	5356	5326	5364	-8	4	-4	A	N
ATOM	870	C	LYS	A	405	6.769	1.261	-4.246	1.00	38.52		A	C
ANISOU	870	C	LYS	A	405	4883	4889	4860	-14	14	17	A	C
ATOM	871	O	LYS	A	405	7.845	1.871	-4.138	1.00	39.60		A	O
ANISOU	871	O	LYS	A	405	5074	5020	4951	-67	-31	27	A	O
ATOM	872	N	PRO	A	411	11.378	8.719	-6.162	1.00	40.98		A	N
ANISOU	872	N	PRO	A	411	5233	5183	5151	-5	-34	-11	A	N
ATOM	873	CA	PRO	A	411	12.797	8.823	-5.802	1.00	40.64		A	C
ANISOU	873	CA	PRO	A	411	5174	5142	5124	4	5	2	A	C
ATOM	875	CB	PRO	A	411	13.365	9.790	-6.851	1.00	40.99		A	C
ANISOU	875	CB	PRO	A	411	5210	5178	5185	23	4	10	A	C
ATOM	878	CG	PRO	A	411	12.282	9.980	-7.899	1.00	40.96		A	C
ANISOU	878	CG	PRO	A	411	5224	5201	5137	-2	2	-8	A	C
ATOM	881	CD	PRO	A	411	11.139	9.090	-7.564	1.00	41.62		A	C
ANISOU	881	CD	PRO	A	411	5289	5269	5254	-8	-22	12	A	C
ATOM	884	C	PRO	A	411	12.963	9.423	-4.413	1.00	40.01		A	C
ANISOU	884	C	PRO	A	411	5102	5063	5037	22	0	18	A	C
ATOM	885	O	PRO	A	411	13.842	9.024	-3.649	1.00	40.41		A	O
ANISOU	885	O	PRO	A	411	5152	5133	5068	14	-16	23	A	O
ATOM	886	N	ALA	A	412	12.110	10.393	-4.103	1.00	38.99		A	N
ANISOU	886	N	ALA	A	412	5004	4941	4870	16	2	37	A	N
ATOM	888	CA	ALA	A	412	12.153	11.073	-2.822	1.00	38.41		A	C
ANISOU	888	CA	ALA	A	412	4916	4852	4825	0	2	38	A	C
ATOM	890	CB	ALA	A	412	11.228	12.266	-2.834	1.00	38.73		A	C
ANISOU	890	CB	ALA	A	412	4960	4896	4859	13	-2	25	A	C
ATOM	894	C	ALA	A	412	11.753	10.126	-1.701	1.00	37.76		A	C
ANISOU	894	C	ALA	A	412	4848	4767	4731	-24	0	33	A	C
ATOM	895	O	ALA	A	412	12.110	10.356	-0.548	1.00	37.49		A	O
ANISOU	895	O	ALA	A	412	4863	4724	4655	-44	-19	89	A	O
ATOM	896	N	LEU	A	413	11.004	9.081	-2.044	1.00	36.91		A	N
ANISOU	896	N	LEU	A	413	4751	4659	4612	-9	15	68	A	N
ATOM	898	CA	LEU	A	413	10.512	8.119	-1.037	1.00	36.37		A	C
ANISOU	898	CA	LEU	A	413	4655	4604	4559	-7	14	40	A	C
ATOM	900	CB	LEU	A	413	9.552	7.102	-1.659	1.00	36.47		A	C
ANISOU	900	CB	LEU	A	413	4689	4608	4558	-7	14	16	A	C
ATOM	903	CG	LEU	A	413	8.095	7.561	-1.688	1.00	37.82		A	C
ANISOU	903	CG	LEU	A	413	4787	4837	4745	-2	-8	11	A	C
ATOM	905	CD1	LEU	A	413	7.993	8.954	-2.281	1.00	39.53		A	C
ANISOU	905	CD1	LEU	A	413	5055	4948	5015	-6	-8	-4	A	C
ATOM	909	CD2	LEU	A	413	7.181	6.580	-2.431	1.00	37.99		A	C
ANISOU	909	CD2	LEU	A	413	4845	4792	4794	12	-19	8	A	C
ATOM	913	C	LEU	A	413	11.670	7.409	-0.373	1.00	35.62		A	C
ANISOU	913	C	LEU	A	413	4572	4493	4468	-7	21	20	A	C
ATOM	914	O	LEU	A	413	11.699	7.241	0.853	1.00	34.40		A	O
ANISOU	914	O	LEU	A	413	4493	4289	4288	2	21	42	A	O
ATOM	915	N	LYS	A	414	12.614	6.971	-1.192	1.00	35.29		A	N
ANISOU	915	N	LYS	A	414	4541	4464	4403	-1	28	38	A	N
ATOM	917	CA	LYS	A	414	13.820	6.347	-0.688	1.00	35.37		A	C
ANISOU	917	CA	LYS	A	414	4523	4458	4458	0	19	12	A	C
ATOM	919	CB	LYS	A	414	14.723	5.907	-1.847	1.00	35.71		A	C
ANISOU	919	CB	LYS	A	414	4587	4484	4495	-10	64	50	A	C

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Figure 1A – 15

ATOM	922	CG	LYS A 414	16.135	5.574	-1.420	1.00	37.41		A	C
ANISOU	922	CG	LYS A 414	4719	4728	4768	-11	-35	23	A	C
ATOM	925	CD	LYS A 414	17.004	5.150	-2.601	1.00	40.21		A	C
ANISOU	925	CD	LYS A 414	5144	5121	5013	5	66	-25	A	C
ATOM	928	CE	LYS A 414	18.459	4.915	-2.180	1.00	41.90		A	C
ANISOU	928	CE	LYS A 414	5258	5352	5309	13	-12	-11	A	C
ATOM	931	NZ	LYS A 414	19.347	6.092	-2.442	1.00	43.26		A	N
ANISOU	931	NZ	LYS A 414	5558	5426	5451	-31	24	4	A	N
ATOM	935	C	LYS A 414	14.563	7.328	0.207	1.00	34.53		A	C
ANISOU	935	C	LYS A 414	4435	4324	4358	4	23	30	A	C
ATOM	936	O	LYS A 414	14.970	6.994	1.319	1.00	33.85		A	O
ANISOU	936	O	LYS A 414	4367	4203	4291	36	28	78	A	O
ATOM	937	N	ASP A 415	14.722	8.560	-0.263	1.00	33.67		A	N
ANISOU	937	N	ASP A 415	4340	4251	4201	-12	31	41	A	N
ATOM	939	CA	ASP A 415	15.480	9.528	0.510	1.00	33.39		A	C
ANISOU	939	CA	ASP A 415	4285	4214	4186	8	42	20	A	C
ATOM	941	CB	ASP A 415	15.760	10.798	-0.306	1.00	34.47		A	C
ANISOU	941	CB	ASP A 415	4441	4315	4341	-27	11	28	A	C
ATOM	944	CG	ASP A 415	16.726	10.547	-1.466	1.00	38.26		A	C
ANISOU	944	CG	ASP A 415	4879	4918	4740	1	118	-30	A	C
ATOM	945	OD1	ASP A 415	17.851	10.032	-1.235	1.00	42.36		A	O
ANISOU	945	OD1	ASP A 415	5221	5501	5372	106	0	-3	A	O
ATOM	946	OD2	ASP A 415	16.434	10.834	-2.648	1.00	42.73		A	O
ANISOU	946	OD2	ASP A 415	5562	5567	5106	42	-10	113	A	O
ATOM	947	C	ASP A 415	14.779	9.851	1.827	1.00	31.24		A	C
ANISOU	947	C	ASP A 415	4006	3913	3949	-27	22	61	A	C
ATOM	948	O	ASP A 415	15.429	10.024	2.834	1.00	30.16		A	O
ANISOU	948	O	ASP A 415	3883	3787	3789	-72	94	86	A	O
ATOM	949	N	GLU A 416	13.455	9.920	1.812	1.00	30.13		A	N
ANISOU	949	N	GLU A 416	3944	3744	3757	0	38	37	A	N
ATOM	951	CA	GLU A 416	12.716	10.197	3.038	1.00	29.50		A	C
ANISOU	951	CA	GLU A 416	3848	3656	3703	13	12	27	A	C
ATOM	953	CB	GLU A 416	11.251	10.525	2.724	1.00	30.55		A	C
ANISOU	953	CB	GLU A 416	3940	3833	3834	6	16	-48	A	C
ATOM	956	CG	GLU A 416	11.081	11.934	2.163	1.00	33.70		A	C
ANISOU	956	CG	GLU A 416	4413	4132	4256	39	48	65	A	C
ATOM	959	CD	GLU A 416	9.809	12.133	1.360	1.00	38.35		A	C
ANISOU	959	CD	GLU A 416	4785	4958	4828	42	-61	-23	A	C
ATOM	960	OE1	GLU A 416	9.231	11.131	0.892	1.00	41.77		A	O
ANISOU	960	OE1	GLU A 416	5241	5212	5417	-93	-38	-23	A	O
ATOM	961	OE2	GLU A 416	9.390	13.306	1.167	1.00	41.60		A	O
ANISOU	961	OE2	GLU A 416	5391	5138	5276	93	-48	22	A	O
ATOM	962	C	GLU A 416	12.814	9.024	4.021	1.00	28.04		A	C
ANISOU	962	C	GLU A 416	3698	3473	3482	0	4	19	A	C
ATOM	963	O	GLU A 416	12.901	9.227	5.234	1.00	27.68		A	O
ANISOU	963	O	GLU A 416	3827	3256	3433	23	26	-16	A	O
ATOM	964	N	LEU A 417	12.799	7.800	3.511	1.00	26.85		A	N
ANISOU	964	N	LEU A 417	3543	3387	3269	64	-16	26	A	N
ATOM	966	CA	LEU A 417	12.905	6.631	4.396	1.00	26.81		A	C
ANISOU	966	CA	LEU A 417	3506	3343	3335	4	33	10	A	C
ATOM	968	CB	LEU A 417	12.668	5.320	3.623	1.00	26.95		A	C
ANISOU	968	CB	LEU A 417	3506	3390	3343	0	38	2	A	C
ATOM	971	CG	LEU A 417	12.746	4.016	4.419	1.00	28.59		A	C
ANISOU	971	CG	LEU A 417	3709	3541	3611	22	-10	24	A	C
ATOM	973	CD1	LEU A 417	11.851	2.964	3.781	1.00	29.15		A	C
ANISOU	973	CD1	LEU A 417	3737	3705	3632	-26	17	-3	A	C
ATOM	977	CD2	LEU A 417	14.175	3.501	4.501	1.00	30.16		A	C
ANISOU	977	CD2	LEU A 417	3801	3846	3810	12	38	7	A	C
ATOM	981	C	LEU A 417	14.287	6.621	5.056	1.00	27.15		A	C
ANISOU	981	C	LEU A 417	3547	3365	3402	32	23	6	A	C
ATOM	982	O	LEU A 417	14.425	6.379	6.265	1.00	26.82		A	O
ANISOU	982	O	LEU A 417	3523	3311	3355	106	32	39	A	O

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Figure 1A – 16

ATOM	983	N	LEU A 418	15.319	6.871	4.260	1.00	27.28		A	N
ANISOU	983	N	LEU A 418	3550	3415	3398	42	55	40	A	N
ATOM	985	CA	LEU A 418	16.664	6.932	4.782	1.00	28.06		A	C
ANISOU	985	CA	LEU A 418	3581	3563	3515	0	45	4	A	C
ATOM	987	CB	LEU A 418	17.694	7.066	3.656	1.00	28.97		A	C
ANISOU	987	CB	LEU A 418	3670	3743	3593	20	55	41	A	C
ATOM	990	CG	LEU A 418	17.860	5.802	2.809	1.00	31.42		A	C
ANISOU	990	CG	LEU A 418	4029	3937	3971	-22	16	-41	A	C
ATOM	992	CD1	LEU A 418	18.713	6.106	1.591	1.00	33.20		A	C
ANISOU	992	CD1	LEU A 418	4211	4246	4155	25	77	2	A	C
ATOM	996	CD2	LEU A 418	18.460	4.636	3.603	1.00	33.05		A	C
ANISOU	996	CD2	LEU A 418	4173	4202	4182	43	13	29	A	C
ATOM	1000	C	LEU A 418	16.834	8.062	5.782	1.00	27.55		A	C
ANISOU	1000	C	LEU A 418	3485	3493	3488	21	57	17	A	C
ATOM	1001	O	LEU A 418	17.539	7.901	6.770	1.00	28.36		A	O
ANISOU	1001	O	LEU A 418	3477	3677	3621	63	57	0	A	O
ATOM	1002	N	ALA A 419	16.193	9.202	5.535	1.00	27.12		A	N
ANISOU	1002	N	ALA A 419	3469	3442	3394	11	33	0	A	N
ATOM	1004	CA	ALA A 419	16.284	10.312	6.479	1.00	26.66		A	C
ANISOU	1004	CA	ALA A 419	3387	3392	3349	22	30	6	A	C
ATOM	1006	CB	ALA A 419	15.624	11.551	5.929	1.00	26.48		A	C
ANISOU	1006	CB	ALA A 419	3339	3340	3381	18	32	-2	A	C
ATOM	1010	C	ALA A 419	15.613	9.895	7.791	1.00	25.80		A	C
ANISOU	1010	C	ALA A 419	3250	3300	3250	51	26	-5	A	C
ATOM	1011	O	ALA A 419	16.109	10.200	8.866	1.00	25.16		A	O
ANISOU	1011	O	ALA A 419	3090	3272	3197	155	109	-111	A	O
ATOM	1012	N	GLU A 420	14.471	9.226	7.681	1.00	25.23		A	N
ANISOU	1012	N	GLU A 420	3229	3169	3189	78	17	-13	A	N
ATOM	1014	CA	GLU A 420	13.755	8.762	8.854	1.00	25.11		A	C
ANISOU	1014	CA	GLU A 420	3210	3159	3170	61	7	-17	A	C
ATOM	1016	CB	GLU A 420	12.405	8.159	8.458	1.00	25.42		A	C
ANISOU	1016	CB	GLU A 420	3225	3184	3249	70	-8	-27	A	C
ATOM	1019	CG	GLU A 420	11.552	7.654	9.611	1.00	25.83		A	C
ANISOU	1019	CG	GLU A 420	3438	3116	3259	102	34	-16	A	C
ATOM	1022	CD	GLU A 420	10.156	7.254	9.165	1.00	27.87		A	C
ANISOU	1022	CD	GLU A 420	3471	3341	3777	123	29	53	A	C
ATOM	1023	OE1	GLU A 420	9.863	7.392	7.966	1.00	32.69		A	O
ANISOU	1023	OE1	GLU A 420	4089	4139	4190	-23	-102	42	A	O
ATOM	1024	OE2	GLU A 420	9.348	6.776	10.004	1.00	31.18		A	O
ANISOU	1024	OE2	GLU A 420	3634	3862	4349	233	156	193	A	O
ATOM	1025	C	GLU A 420	14.624	7.774	9.628	1.00	25.06		A	C
ANISOU	1025	C	GLU A 420	3219	3157	3145	100	0	-12	A	C
ATOM	1026	O	GLU A 420	14.710	7.831	10.856	1.00	24.72		A	O
ANISOU	1026	O	GLU A 420	3167	3153	3072	139	-67	16	A	O
ATOM	1027	N	ALA A 421	15.280	6.868	8.921	1.00	25.14		A	N
ANISOU	1027	N	ALA A 421	3210	3235	3104	93	6	2	A	N
ATOM	1029	CA	ALA A 421	16.197	5.961	9.610	1.00	26.00		A	C
ANISOU	1029	CA	ALA A 421	3323	3272	3282	101	9	-1	A	C
ATOM	1031	CB	ALA A 421	16.768	4.947	8.634	1.00	26.21		A	C
ANISOU	1031	CB	ALA A 421	3393	3290	3275	99	12	6	A	C
ATOM	1035	C	ALA A 421	17.341	6.720	10.311	1.00	26.64		A	C
ANISOU	1035	C	ALA A 421	3377	3391	3352	103	31	-42	A	C
ATOM	1036	O	ALA A 421	17.751	6.334	11.415	1.00	28.07		A	O
ANISOU	1036	O	ALA A 421	3569	3618	3477	176	38	-31	A	O
ATOM	1037	N	ASN A 422	17.861	7.779	9.690	1.00	27.50		A	N
ANISOU	1037	N	ASN A 422	3447	3513	3488	87	59	-59	A	N
ATOM	1039	CA	ASN A 422	18.946	8.572	10.299	1.00	27.66		A	C
ANISOU	1039	CA	ASN A 422	3481	3578	3447	36	23	-53	A	C
ATOM	1041	CB	ASN A 422	19.520	9.665	9.371	1.00	29.05		A	C
ANISOU	1041	CB	ASN A 422	3614	3734	3690	16	31	-2	A	C
ATOM	1044	CG	AASN A 422	19.968	9.100	8.023	0.50	29.62		A	C
ANISOU	1044	CG	AASN A 422	3749	3779	3724	0	15	-46	A	C



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Figure 1A – 17

ATOM	1045	CG	BASN	A	422	19.813	10.941	10.137	0.50	30.30		A	C
ANISOU	1045	CG	BASN	A	422	3857	3854	3799	-31	34	-30	A	C
ATOM	1046	OD1	AASN	A	422	20.391	7.948	7.919	0.50	30.25		A	O
ANISOU	1046	OD1	AASN	A	422	3759	3861	3873	14	-29	-22	A	O
ATOM	1047	OD1	BASN	A	422	20.833	11.032	10.831	0.50	32.65		A	O
ANISOU	1047	OD1	BASN	A	422	4039	4232	4131	17	-74	23	A	O
ATOM	1048	ND2	AASN	A	422	19.951	9.951	6.996	0.50	31.70		A	N
ANISOU	1048	ND2	AASN	A	422	4007	4094	3941	-12	27	60	A	N
ATOM	1049	ND2	BASN	A	422	18.962	11.949	9.980	0.50	32.73		A	N
ANISOU	1049	ND2	BASN	A	422	4118	4161	4154	54	52	55	A	N
ATOM	1054	C	ASN	A	422	18.504	9.180	11.642	1.00	26.58		A	C
ANISOU	1054	C	ASN	A	422	3268	3475	3352	56	26	-58	A	C
ATOM	1055	O	ASN	A	422	19.305	9.253	12.595	1.00	26.92		A	O
ANISOU	1055	O	ASN	A	422	3269	3702	3256	135	53	-125	A	O
ATOM	1056	N	VAL	A	423	17.237	9.581	11.733	1.00	24.25		A	N
ANISOU	1056	N	VAL	A	423	3086	3115	3011	46	-32	-13	A	N
ATOM	1058	CA	VAL	A	423	16.707	10.074	13.002	1.00	23.09		A	C
ANISOU	1058	CA	VAL	A	423	2848	2936	2989	32	-8	-41	A	C
ATOM	1060	CB	VAL	A	423	15.373	10.801	12.814	1.00	22.10		A	C
ANISOU	1060	CB	VAL	A	423	2755	2841	2799	2	-43	-50	A	C
ATOM	1062	CG1	VAL	A	423	14.630	10.944	14.159	1.00	21.29		A	C
ANISOU	1062	CG1	VAL	A	423	2626	2676	2784	57	-75	48	A	C
ATOM	1066	CG2	VAL	A	423	15.599	12.158	12.190	1.00	22.62		A	C
ANISOU	1066	CG2	VAL	A	423	2677	2983	2932	58	-49	18	A	C
ATOM	1070	C	VAL	A	423	16.520	8.923	13.997	1.00	22.41		A	C
ANISOU	1070	C	VAL	A	423	2734	2908	2873	46	-4	-48	A	C
ATOM	1071	O	VAL	A	423	17.001	8.983	15.125	1.00	22.33		A	O
ANISOU	1071	O	VAL	A	423	2652	2880	2951	7	-4	-124	A	O
ATOM	1072	N	MET	A	424	15.841	7.858	13.576	1.00	22.10		A	N
ANISOU	1072	N	MET	A	424	2741	2788	2867	62	-2	-44	A	N
ATOM	1074	CA	MET	A	424	15.536	6.772	14.491	1.00	22.26		A	C
ANISOU	1074	CA	MET	A	424	2807	2826	2825	54	-37	-48	A	C
ATOM	1076	CB	MET	A	424	14.652	5.707	13.840	1.00	22.00		A	C
ANISOU	1076	CB	MET	A	424	2776	2743	2839	60	1	-62	A	C
ATOM	1079	CG	AMET	A	424	13.255	6.300	13.543	0.60	21.20		A	C
ANISOU	1079	CG	AMET	A	424	2667	2706	2680	-48	-63	-27	A	C
ATOM	1080	CG	BMET	A	424	13.327	6.107	13.327	0.40	22.55		A	C
ANISOU	1080	CG	BMET	A	424	2829	2858	2880	1	-24	-2	A	C
ATOM	1085	SD	AMET	A	424	12.014	5.153	12.950	0.60	19.70		A	S
ANISOU	1085	SD	AMET	A	424	2334	2730	2420	113	-69	-212	A	S
ATOM	1086	SD	BMET	A	424	12.626	7.152	14.450	0.40	22.97		A	S
ANISOU	1086	SD	BMET	A	424	2777	2849	3100	0	-30	-62	A	S
ATOM	1087	CE	AMET	A	424	11.607	4.228	14.400	0.60	22.13		A	C
ANISOU	1087	CE	AMET	A	424	2670	2942	2795	19	-36	40	A	C
ATOM	1088	CE	BMET	A	424	12.186	6.091	15.801	0.40	24.48		A	C
ANISOU	1088	CE	BMET	A	424	3077	3086	3137	12	-1	8	A	C
ATOM	1095	C	MET	A	424	16.789	6.103	15.049	1.00	22.87		A	C
ANISOU	1095	C	MET	A	424	2927	2845	2917	47	-68	-25	A	C
ATOM	1096	O	MET	A	424	16.761	5.630	16.169	1.00	22.05		A	O
ANISOU	1096	O	MET	A	424	2905	2682	2791	203	-215	-62	A	O
ATOM	1097	N	GLN	A	425	17.880	6.102	14.305	1.00	24.34		A	N
ANISOU	1097	N	GLN	A	425	3117	3080	3050	95	-43	-33	A	N
ATOM	1099	CA	GLN	A	425	19.067	5.393	14.791	1.00	26.33		A	C
ANISOU	1099	CA	GLN	A	425	3303	3342	3356	75	-34	-14	A	C
ATOM	1101	CB	GLN	A	425	20.153	5.262	13.720	1.00	27.41		A	C
ANISOU	1101	CB	GLN	A	425	3431	3551	3432	68	-24	9	A	C
ATOM	1104	CG	AGLN	A	425	20.788	6.597	13.484	0.70	29.50		A	C
ANISOU	1104	CG	AGLN	A	425	3760	3659	3790	5	13	21	A	C
ATOM	1105	CG	BGLN	A	425	20.281	3.786	13.371	0.30	28.89		A	C
ANISOU	1105	CG	BGLN	A	425	3699	3612	3663	-18	8	-6	A	C
ATOM	1110	CD	AGLN	A	425	21.697	6.569	12.252	0.70	32.72		A	C
ANISOU	1110	CD	AGLN	A	425	4159	4184	4086	10	126	25	A	C

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Figure 1A – 18

ATOM	1111	CD	BGLN	A	425	21.620	3.213	13.791	0.30	30.99		A	C
ANISOU	1111	CD	BGLN	A	425	3847	3937	3989	25	-23	-7	A	C
ATOM	1112	OE1	AGLN	A	425	21.901	5.508	11.642	0.70	34.07		A	O
ANISOU	1112	OE1	AGLN	A	425	4346	4305	4293	-9	156	-42	A	O
ATOM	1113	OE1	BGLN	A	425	21.693	2.397	14.716	0.30	32.57		A	O
ANISOU	1113	OE1	BGLN	A	425	4132	4119	4124	18	11	40	A	O
ATOM	1114	NE2	AGLN	A	425	22.236	7.725	11.886	0.70	33.74		A	N
ANISOU	1114	NE2	AGLN	A	425	4229	4266	4323	-103	63	69	A	N
ATOM	1115	NE2	BGLN	A	425	22.687	3.640	13.118	0.30	32.33		A	N
ANISOU	1115	NE2	BGLN	A	425	4079	4122	4081	-36	58	25	A	N
ATOM	1120	C	GLN	A	425	19.629	6.028	16.037	1.00	26.36		A	C
ANISOU	1120	C	GLN	A	425	3298	3372	3346	88	-30	-3	A	C
ATOM	1121	O	GLN	A	425	20.365	5.388	16.792	1.00	26.84		A	O
ANISOU	1121	O	GLN	A	425	3253	3552	3391	233	38	14	A	O
ATOM	1122	N	GLN	A	426	19.241	7.277	16.268	1.00	25.74		A	N
ANISOU	1122	N	GLN	A	426	3168	3276	3334	98	10	-26	A	N
ATOM	1124	CA	GLN	A	426	19.777	8.048	17.367	1.00	25.85		A	C
ANISOU	1124	CA	GLN	A	426	3222	3275	3323	99	-23	1	A	C
ATOM	1126	CB	GLN	A	426	19.975	9.499	16.909	1.00	26.12		A	C
ANISOU	1126	CB	GLN	A	426	3285	3277	3363	64	0	0	A	C
ATOM	1129	CG	AGLN	A	426	20.843	9.624	15.652	0.60	27.31		A	C
ANISOU	1129	CG	AGLN	A	426	3378	3542	3453	55	21	-11	A	C
ATOM	1130	CG	BGLN	A	426	20.896	9.633	15.752	0.40	26.22		A	C
ANISOU	1130	CG	BGLN	A	426	3278	3350	3335	47	-12	10	A	C
ATOM	1135	CD	AGLN	A	426	20.984	11.052	15.138	0.60	28.35		A	C
ANISOU	1135	CD	AGLN	A	426	3452	3649	3668	41	63	-9	A	C
ATOM	1136	CD	BGLN	A	426	22.273	9.162	16.128	0.40	26.12		A	C
ANISOU	1136	CD	BGLN	A	426	3252	3349	3324	19	-62	5	A	C
ATOM	1137	OE1	AGLN	A	426	21.486	11.917	15.850	0.60	31.37		A	O
ANISOU	1137	OE1	AGLN	A	426	3780	4058	4079	-70	11	-158	A	O
ATOM	1138	OE1	BGLN	A	426	22.619	9.155	17.314	0.40	25.67		A	O
ANISOU	1138	OE1	BGLN	A	426	3168	3283	3300	34	-43	-2	A	O
ATOM	1139	NE2	AGLN	A	426	20.521	11.305	13.914	0.60	28.60		A	N
ANISOU	1139	NE2	AGLN	A	426	3591	3748	3525	-25	185	-70	A	N
ATOM	1140	NE2	BGLN	A	426	23.056	8.751	15.143	0.40	27.26		A	N
ANISOU	1140	NE2	BGLN	A	426	3398	3526	3435	-15	-30	13	A	N
ATOM	1145	C	GLN	A	426	18.909	8.006	18.610	1.00	25.45		A	C
ANISOU	1145	C	GLN	A	426	3175	3236	3257	93	-51	-16	A	C
ATOM	1146	O	GLN	A	426	19.305	8.526	19.655	1.00	26.56		A	O
ANISOU	1146	O	GLN	A	426	3269	3428	3393	215	-123	-121	A	O
ATOM	1147	N	LEU	A	427	17.753	7.365	18.513	1.00	24.49		A	N
ANISOU	1147	N	LEU	A	427	3108	3068	3130	106	-42	39	A	N
ATOM	1149	CA	LEU	A	427	16.789	7.382	19.586	1.00	23.86		A	C
ANISOU	1149	CA	LEU	A	427	2970	3061	3035	50	-55	-14	A	C
ATOM	1151	CB	LEU	A	427	15.416	7.783	19.030	1.00	23.27		A	C
ANISOU	1151	CB	LEU	A	427	2885	2981	2976	89	-32	-42	A	C
ATOM	1154	CG	LEU	A	427	15.417	9.062	18.198	1.00	22.67		A	C
ANISOU	1154	CG	LEU	A	427	2763	3003	2846	35	-19	-48	A	C
ATOM	1156	CD1	LEU	A	427	13.993	9.272	17.634	1.00	24.63		A	C
ANISOU	1156	CD1	LEU	A	427	2945	3300	3110	110	-115	-19	A	C
ATOM	1160	CD2	LEU	A	427	15.910	10.276	18.960	1.00	21.36		A	C
ANISOU	1160	CD2	LEU	A	427	2587	2681	2848	142	112	82	A	C
ATOM	1164	C	LEU	A	427	16.688	6.046	20.304	1.00	24.23		A	C
ANISOU	1164	C	LEU	A	427	3014	3104	3086	68	-14	-19	A	C
ATOM	1165	O	LEU	A	427	16.588	4.992	19.680	1.00	26.16		A	O
ANISOU	1165	O	LEU	A	427	3464	3231	3241	103	-17	-23	A	O
ATOM	1166	N	ASP	A	428	16.705	6.110	21.630	1.00	23.52		A	N
ANISOU	1166	N	ASP	A	428	2825	3072	3037	141	-74	1	A	N
ATOM	1168	CA	ASP	A	428	16.571	4.945	22.458	1.00	23.68		A	C
ANISOU	1168	CA	ASP	A	428	2856	3062	3078	72	-17	4	A	C
ATOM	1170	CB	ASP	A	428	17.973	4.393	22.747	1.00	24.45		A	C
ANISOU	1170	CB	ASP	A	428	2888	3184	3217	89	-14	41	A	C

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## Figure 1A – 19

ATOM	1173	CG	AASP	A	428	17.964	3.135	23.612	0.50	25.86		A	C
ANISOU	1173	CG	AASP	A	428	3208	3249	3367	71	40	36	A	C
ATOM	1174	CG	BASP	A	428	17.955	3.298	23.773	0.50	26.42		A	C
ANISOU	1174	CG	BASP	A	428	3311	3294	3430	53	27	51	A	C
ATOM	1175	OD1	AASP	A	428	17.062	2.963	24.462	0.50	26.81		A	O
ANISOU	1175	OD1	AASP	A	428	3276	3409	3498	61	159	66	A	O
ATOM	1176	OD1	BASP	A	428	17.068	2.409	23.673	0.50	26.12		A	O
ANISOU	1176	OD1	BASP	A	428	3276	3213	3435	67	5	-47	A	O
ATOM	1177	OD2	AASP	A	428	18.857	2.255	23.519	0.50	26.18		A	O
ANISOU	1177	OD2	AASP	A	428	3190	3357	3397	145	124	-90	A	O
ATOM	1178	OD2	BASP	A	428	18.787	3.274	24.724	0.50	28.78		A	O
ANISOU	1178	OD2	BASP	A	428	3718	3669	3546	48	-102	-27	A	O
ATOM	1179	C	ASP	A	428	15.849	5.337	23.735	1.00	21.84		A	C
ANISOU	1179	C	ASP	A	428	2608	2803	2887	90	-73	39	A	C
ATOM	1180	O	ASP	A	428	16.400	5.968	24.641	1.00	22.32		A	O
ANISOU	1180	O	ASP	A	428	2367	3020	3093	123	-142	16	A	O
ATOM	1181	N	ASN	A	429	14.568	5.020	23.768	1.00	19.55		A	N
ANISOU	1181	N	ASN	A	429	2392	2449	2587	91	-51	52	A	N
ATOM	1183	CA	ASN	A	429	13.717	5.357	24.886	1.00	19.12		A	C
ANISOU	1183	CA	ASN	A	429	2430	2405	2430	69	-60	45	A	C
ATOM	1185	CB	ASN	A	429	13.159	6.762	24.718	1.00	17.77		A	C
ANISOU	1185	CB	ASN	A	429	2318	2185	2249	24	-23	28	A	C
ATOM	1188	CG	ASN	A	429	12.258	7.183	25.870	1.00	17.98		A	C
ANISOU	1188	CG	ASN	A	429	2258	2194	2380	82	22	108	A	C
ATOM	1189	OD1	ASN	A	429	11.034	7.055	25.796	1.00	16.43		A	O
ANISOU	1189	OD1	ASN	A	429	2098	2054	2090	98	-32	83	A	O
ATOM	1190	ND2	ASN	A	429	12.865	7.691	26.943	1.00	20.08		A	N
ANISOU	1190	ND2	ASN	A	429	2601	2375	2654	40	3	122	A	N
ATOM	1193	C	ASN	A	429	12.565	4.370	24.907	1.00	18.21		A	C
ANISOU	1193	C	ASN	A	429	2270	2242	2403	113	-43	29	A	C
ATOM	1194	O	ASN	A	429	12.090	3.935	23.855	1.00	18.09		A	O
ANISOU	1194	O	ASN	A	429	2283	2218	2369	264	-134	138	A	O
ATOM	1195	N	PRO	A	430	12.094	3.980	26.071	1.00	18.41		A	N
ANISOU	1195	N	PRO	A	430	2353	2231	2411	126	-65	40	A	N
ATOM	1196	CA	PRO	A	430	10.987	3.019	26.102	1.00	18.02		A	C
ANISOU	1196	CA	PRO	A	430	2208	2290	2347	107	-25	37	A	C
ATOM	1198	CB	PRO	A	430	10.798	2.746	27.595	1.00	18.90		A	C
ANISOU	1198	CB	PRO	A	430	2360	2371	2450	49	-64	127	A	C
ATOM	1201	CG	PRO	A	430	12.011	3.216	28.233	1.00	21.00		A	C
ANISOU	1201	CG	PRO	A	430	2603	2659	2715	-33	-78	90	A	C
ATOM	1204	CD	PRO	A	430	12.582	4.316	27.417	1.00	18.91		A	C
ANISOU	1204	CD	PRO	A	430	2336	2358	2489	48	-30	83	A	C
ATOM	1207	C	PRO	A	430	9.655	3.438	25.498	1.00	17.07		A	C
ANISOU	1207	C	PRO	A	430	2133	2097	2252	46	-2	-18	A	C
ATOM	1208	O	PRO	A	430	8.799	2.586	25.242	1.00	15.97		A	O
ANISOU	1208	O	PRO	A	430	1931	1828	2307	128	48	-53	A	O
ATOM	1209	N	TYR	A	431	9.467	4.739	25.329	1.00	15.37		A	N
ANISOU	1209	N	TYR	A	431	1931	1945	1963	129	-57	86	A	N
ATOM	1211	CA	TYR	A	431	8.164	5.249	24.909	1.00	14.91		A	C
ANISOU	1211	CA	TYR	A	431	1863	1917	1885	123	3	-15	A	C
ATOM	1213	CB	TYR	A	431	7.724	6.362	25.887	1.00	15.24		A	C
ANISOU	1213	CB	TYR	A	431	2039	1847	1905	54	17	-27	A	C
ATOM	1216	CG	TYR	A	431	7.691	5.822	27.302	1.00	13.98		A	C
ANISOU	1216	CG	TYR	A	431	1844	1637	1829	228	-2	-110	A	C
ATOM	1217	CD1	TYR	A	431	6.758	4.873	27.665	1.00	15.77		A	C
ANISOU	1217	CD1	TYR	A	431	2030	2006	1956	140	-104	35	A	C
ATOM	1219	CE1	TYR	A	431	6.729	4.338	28.939	1.00	17.24		A	C
ANISOU	1219	CE1	TYR	A	431	2366	2144	2040	4	128	90	A	C
ATOM	1221	CZ	TYR	A	431	7.664	4.746	29.860	1.00	17.61		A	C
ANISOU	1221	CZ	TYR	A	431	2421	2286	1982	181	60	31	A	C
ATOM	1222	OH	TYR	A	431	7.610	4.204	31.161	1.00	21.39		A	O
ANISOU	1222	OH	TYR	A	431	3413	2588	2126	171	88	263	A	O

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ATOM	1224	CE2	TYR	A	431	8.591	5.711	29.537	1.00	18.25		A	C
ANISOU	1224	CE2	TYR	A	431	2447	2414	2071	119	-22	-24	A	C
ATOM	1226	CD2	TYR	A	431	8.613	6.244	28.257	1.00	16.88		A	C
ANISOU	1226	CD2	TYR	A	431	2260	2085	2067	129	17	-95	A	C
ATOM	1228	C	TYR	A	431	8.207	5.714	23.472	1.00	15.69		A	C
ANISOU	1228	C	TYR	A	431	2034	1970	1957	109	15	24	A	C
ATOM	1229	O	TYR	A	431	7.359	6.483	23.046	1.00	15.03		A	O
ANISOU	1229	O	TYR	A	431	2052	1759	1899	181	43	72	A	O
ATOM	1230	N	ILE	A	432	9.166	5.180	22.716	1.00	16.31		A	N
ANISOU	1230	N	ILE	A	432	2030	2089	2076	142	3	74	A	N
ATOM	1232	CA	ILE	A	432	9.264	5.441	21.296	1.00	17.77		A	C
ANISOU	1232	CA	ILE	A	432	2344	2220	2184	57	-1	11	A	C
ATOM	1234	CB	ILE	A	432	10.462	6.361	21.011	1.00	19.50		A	C
ANISOU	1234	CB	ILE	A	432	2391	2568	2449	76	36	17	A	C
ATOM	1236	CG1	ILE	A	432	10.193	7.751	21.567	1.00	21.66		A	C
ANISOU	1236	CG1	ILE	A	432	2909	2681	2637	-43	-61	-47	A	C
ATOM	1239	CD1	ILE	A	432	11.357	8.722	21.534	1.00	24.92		A	C
ANISOU	1239	CD1	ILE	A	432	3014	3242	3210	5	-27	12	A	C
ATOM	1243	CG2	ILE	A	432	10.732	6.409	19.557	1.00	21.52		A	C
ANISOU	1243	CG2	ILE	A	432	2846	2749	2579	-80	-37	108	A	C
ATOM	1247	C	ILE	A	432	9.428	4.121	20.586	1.00	18.15		A	C
ANISOU	1247	C	ILE	A	432	2347	2335	2212	139	55	-20	A	C
ATOM	1248	O	ILE	A	432	10.124	3.257	21.095	1.00	19.70		A	O
ANISOU	1248	O	ILE	A	432	2928	2381	2172	354	78	-46	A	O
ATOM	1249	N	VAL	A	433	8.754	3.962	19.445	1.00	17.90		A	N
ANISOU	1249	N	VAL	A	433	2424	2120	2256	43	5	-16	A	N
ATOM	1251	CA	VAL	A	433	8.908	2.772	18.599	1.00	18.44		A	C
ANISOU	1251	CA	VAL	A	433	2432	2221	2350	99	40	15	A	C
ATOM	1253	CB	VAL	A	433	7.858	2.755	17.494	1.00	19.40		A	C
ANISOU	1253	CB	VAL	A	433	2680	2288	2400	21	-2	-42	A	C
ATOM	1255	CG1	VAL	A	433	8.180	1.675	16.457	1.00	20.05		A	C
ANISOU	1255	CG1	VAL	A	433	2858	2429	2328	140	-17	-33	A	C
ATOM	1259	CG2	VAL	A	433	6.494	2.567	18.094	1.00	19.95		A	C
ANISOU	1259	CG2	VAL	A	433	2735	2401	2444	151	-109	54	A	C
ATOM	1263	C	VAL	A	433	10.309	2.792	18.017	1.00	19.95		A	C
ANISOU	1263	C	VAL	A	433	2678	2416	2486	34	159	-12	A	C
ATOM	1264	O	VAL	A	433	10.670	3.679	17.253	1.00	22.17		A	O
ANISOU	1264	O	VAL	A	433	3087	2545	2791	247	406	43	A	O
ATOM	1265	N	ARG	A	434	11.100	1.815	18.405	1.00	20.13		A	N
ANISOU	1265	N	ARG	A	434	2583	2571	2494	67	52	-14	A	N
ATOM	1267	CA	ARG	A	434	12.508	1.735	17.990	1.00	21.52		A	C
ANISOU	1267	CA	ARG	A	434	2738	2743	2694	-31	89	-80	A	C
ATOM	1269	CB	ARG	A	434	13.356	0.942	18.990	1.00	23.23		A	C
ANISOU	1269	CB	ARG	A	434	2933	3006	2886	24	47	-47	A	C
ATOM	1272	CG	AARG	A	434	13.818	1.713	20.205	0.50	26.39		A	C
ANISOU	1272	CG	AARG	A	434	3357	3317	3352	-47	-11	-158	A	C
ATOM	1273	CG	BARG	A	434	13.771	1.735	20.280	0.50	23.87		A	C
ANISOU	1273	CG	BARG	A	434	3062	3007	3000	-45	63	-79	A	C
ATOM	1278	CD	AARG	A	434	13.448	1.075	21.528	0.50	30.79		A	C
ANISOU	1278	CD	AARG	A	434	3933	3987	3776	-49	77	13	A	C
ATOM	1279	CD	BARG	A	434	14.760	0.978	21.209	0.50	25.31		A	C
ANISOU	1279	CD	BARG	A	434	3223	3238	3155	-4	0	51	A	C
ATOM	1284	NE	AARG	A	434	14.426	0.138	22.087	0.50	34.45		A	N
ANISOU	1284	NE	AARG	A	434	4347	4346	4396	62	7	0	A	N
ATOM	1285	NE	BARG	A	434	14.933	1.510	22.583	0.50	26.09		A	N
ANISOU	1285	NE	BARG	A	434	3379	3259	3275	7	49	-73	A	N
ATOM	1288	CZ	AARG	A	434	14.111	-1.015	22.668	0.50	36.93		A	C
ANISOU	1288	CZ	AARG	A	434	4752	4612	4666	-13	48	24	A	C
ATOM	1289	CZ	BARG	A	434	14.261	1.073	23.667	0.50	26.51		A	C
ANISOU	1289	CZ	BARG	A	434	3395	3302	3373	24	20	13	A	C
ATOM	1290	NH1AARG	A	434		12.845	-1.407	22.729	0.50	37.67		A	N
ANISOU	1290	NH1AARG	A	434		4739	4771	4800	-12	4	-9	A	N

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## Figure 1A – 21

ATOM	1291	NH1BARG	A	434	13.328	0.137	23.549	0.50	27.65		A	N	
ANISOU	1291	NH1BARG	A	434	3432	3498	3576	2	16	18	A	N	
ATOM	1296	NH2AARG	A	434	15.061	-1.790	23.174	0.50	38.57		A	N	
ANISOU	1296	NH2AARG	A	434	4869	4903	4883	44	-12	18	A	N	
ATOM	1297	NH2BARG	A	434	14.494	1.593	24.875	0.50	25.81		A	N	
ANISOU	1297	NH2BARG	A	434	3176	3341	3287	117	-14	108	A	N	
ATOM	1302	C	ARG	A	434	12.654	1.130	16.603	1.00	20.63	A	C	
ANISOU	1302	C	ARG	A	434	2599	2642	2596	-4	94	-84	A	C
ATOM	1303	O	ARG	A	434	11.837	0.329	16.167	1.00	20.09	A	O	
ANISOU	1303	O	ARG	A	434	2595	2446	2590	143	172	-73	A	O
ATOM	1304	N	MET	A	435	13.700	1.567	15.917	1.00	20.72	A	N	
ANISOU	1304	N	MET	A	435	2632	2633	2607	-15	137	-127	A	N
ATOM	1306	CA	MET	A	435	14.034	1.003	14.614	1.00	20.26	A	C	
ANISOU	1306	CA	MET	A	435	2560	2635	2501	-15	64	-87	A	C
ATOM	1308	CB	MET	A	435	14.702	2.054	13.712	1.00	21.45	A	C	
ANISOU	1308	CB	MET	A	435	2784	2714	2650	12	78	-67	A	C
ATOM	1311	CG	MET	A	435	15.357	1.448	12.440	1.00	22.57	A	C	
ANISOU	1311	CG	MET	A	435	2914	2870	2791	13	74	-50	A	C
ATOM	1314	SD	MET	A	435	16.134	2.694	11.387	1.00	27.47	A	S	
ANISOU	1314	SD	MET	A	435	3552	3586	3298	-68	433	150	A	S
ATOM	1315	CE	MET	A	435	17.381	3.215	12.364	1.00	27.56	A	C	
ANISOU	1315	CE	MET	A	435	3650	3465	3354	28	93	127	A	C
ATOM	1319	C	MET	A	435	14.962	-0.187	14.840	1.00	20.60	A	C	
ANISOU	1319	C	MET	A	435	2628	2669	2527	-2	70	-56	A	C
ATOM	1320	O	MET	A	435	15.876	-0.131	15.646	1.00	21.00	A	O	
ANISOU	1320	O	MET	A	435	2647	2738	2592	98	96	-171	A	O
ATOM	1321	N	ILE	A	436	14.687	-1.291	14.166	1.00	19.49	A	N	
ANISOU	1321	N	ILE	A	436	2433	2560	2410	-47	66	-45	A	N
ATOM	1323	CA	ILE	A	436	15.563	-2.450	14.196	1.00	20.42	A	C	
ANISOU	1323	CA	ILE	A	436	2601	2601	2554	-4	70	-14	A	C
ATOM	1325	CB	ILE	A	436	14.767	-3.743	13.913	1.00	20.35	A	C	
ANISOU	1325	CB	ILE	A	436	2562	2591	2577	32	70	-32	A	C
ATOM	1327	CG1	ILE	A	436	13.540	-3.849	14.832	1.00	21.20	A	C	
ANISOU	1327	CG1	ILE	A	436	2654	2646	2753	-58	58	55	A	C
ATOM	1330	CD1	ILE	A	436	13.879	-3.891	16.299	1.00	21.90	A	C	
ANISOU	1330	CD1	ILE	A	436	2703	2806	2809	-93	99	-10	A	C
ATOM	1334	CG2	ILE	A	436	15.688	-4.956	14.048	1.00	20.45	A	C	
ANISOU	1334	CG2	ILE	A	436	2669	2455	2646	-19	17	31	A	C
ATOM	1338	C	ILE	A	436	16.638	-2.256	13.133	1.00	20.93	A	C	
ANISOU	1338	C	ILE	A	436	2639	2654	2657	14	76	-34	A	C
ATOM	1339	O	ILE	A	436	17.819	-2.539	13.356	1.00	20.97	A	O	
ANISOU	1339	O	ILE	A	436	2560	2820	2584	43	205	-66	A	O
ATOM	1340	N	GLY	A	437	16.217	-1.791	11.975	1.00	20.87	A	N	
ANISOU	1340	N	GLY	A	437	2704	2622	2601	-15	94	-43	A	N
ATOM	1342	CA	GLY	A	437	17.167	-1.457	10.916	1.00	21.81	A	C	
ANISOU	1342	CA	GLY	A	437	2801	2744	2740	-40	115	-13	A	C
ATOM	1345	C	GLY	A	437	16.498	-1.252	9.580	1.00	22.29	A	C	
ANISOU	1345	C	GLY	A	437	2877	2783	2807	-18	73	5	A	C
ATOM	1346	O	GLY	A	437	15.292	-1.133	9.479	1.00	21.71	A	O	
ANISOU	1346	O	GLY	A	437	2921	2662	2665	24	214	28	A	O
ATOM	1347	N	ILE	A	438	17.294	-1.239	8.514	1.00	23.91	A	N	
ANISOU	1347	N	ILE	A	438	3061	3047	2976	-27	131	-18	A	N
ATOM	1349	CA	ILE	A	438	16.736	-1.070	7.165	1.00	24.89	A	C	
ANISOU	1349	CA	ILE	A	438	3209	3140	3109	0	67	6	A	C
ATOM	1351	CB	ILE	A	438	17.229	0.224	6.485	1.00	25.52	A	C	
ANISOU	1351	CB	ILE	A	438	3337	3149	3210	-10	64	7	A	C
ATOM	1353	CG1	ILE	A	438	18.746	0.288	6.514	1.00	27.81	A	C	
ANISOU	1353	CG1	ILE	A	438	3547	3465	3555	40	28	-16	A	C
ATOM	1356	CD1	ILE	A	438	19.306	1.477	5.727	1.00	29.60	A	C	
ANISOU	1356	CD1	ILE	A	438	3818	3654	3775	-62	75	52	A	C
ATOM	1360	CG2	ILE	A	438	16.606	1.460	7.148	1.00	25.50	A	C	
ANISOU	1360	CG2	ILE	A	438	3390	3192	3107	10	119	24	A	C

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Figure 1A – 22

ATOM	1364	C	ILE A 438	17.139	-2.262	6.315	1.00	24.86		A	C
ANISOU	1364	C	ILE A 438	3200	3205	3038	-40	109	-16	A	C
ATOM	1365	O	ILE A 438	18.120	-2.940	6.597	1.00	25.22		A	O
ANISOU	1365	O	ILE A 438	3371	3290	2921	-41	157	4	A	O
ATOM	1366	N	CYS A 439	16.353	-2.535	5.297	1.00	25.63		A	N
ANISOU	1366	N	CYS A 439	3340	3310	3086	-14	105	-2	A	N
ATOM	1368	CA	CYS A 439	16.662	-3.647	4.424	1.00	26.92		A	C
ANISOU	1368	CA	CYS A 439	3533	3382	3312	23	0	-42	A	C
ATOM	1370	CB	CYS A 439	15.769	-4.838	4.784	1.00	27.10		A	C
ANISOU	1370	CB	CYS A 439	3577	3415	3303	13	47	-24	A	C
ATOM	1373	SG	CYS A 439	16.214	-6.350	3.932	1.00	30.86		A	S
ANISOU	1373	SG	CYS A 439	4346	3590	3787	116	43	-117	A	S
ATOM	1374	C	CYS A 439	16.400	-3.223	2.983	1.00	27.02		A	C
ANISOU	1374	C	CYS A 439	3545	3438	3281	-3	31	-23	A	C
ATOM	1375	O	CYS A 439	15.305	-2.760	2.677	1.00	26.70		A	O
ANISOU	1375	O	CYS A 439	3691	3390	3064	124	93	-101	A	O
ATOM	1376	N	GLU A 440	17.407	-3.400	2.126	1.00	27.06		A	N
ANISOU	1376	N	GLU A 440	3483	3410	3388	19	21	-56	A	N
ATOM	1378	CA	GLU A 440	17.310	-3.139	0.689	1.00	28.12		A	C
ANISOU	1378	CA	GLU A 440	3599	3554	3529	6	36	-24	A	C
ATOM	1380	CB	GLU A 440	18.686	-2.695	0.194	1.00	29.01		A	C
ANISOU	1380	CB	GLU A 440	3687	3648	3688	-8	49	-55	A	C
ATOM	1383	CG	GLU A 440	18.690	-2.030	-1.160	1.00	32.54		A	C
ANISOU	1383	CG	GLU A 440	4222	4131	4009	-6	0	12	A	C
ATOM	1386	CD	GLU A 440	20.088	-1.618	-1.570	1.00	35.97		A	C
ANISOU	1386	CD	GLU A 440	4440	4565	4660	-17	95	8	A	C
ATOM	1387	OE1	GLU A 440	20.987	-1.514	-0.691	1.00	38.32		A	O
ANISOU	1387	OE1	GLU A 440	4844	4832	4881	-35	33	-45	A	O
ATOM	1388	OE2	GLU A 440	20.282	-1.414	-2.778	1.00	39.40		A	O
ANISOU	1388	OE2	GLU A 440	5040	5001	4930	-32	123	80	A	O
ATOM	1389	C	GLU A 440	16.913	-4.436	-0.023	1.00	27.47		A	C
ANISOU	1389	C	GLU A 440	3532	3525	3379	19	46	-18	A	C
ATOM	1390	O	GLU A 440	17.771	-5.263	-0.314	1.00	28.68		A	O
ANISOU	1390	O	GLU A 440	3692	3678	3524	73	46	-53	A	O
ATOM	1391	N	ALA A 441	15.627	-4.642	-0.268	1.00	26.82		A	N
ANISOU	1391	N	ALA A 441	3510	3391	3288	44	83	-6	A	N
ATOM	1393	CA	ALA A 441	15.175	-5.906	-0.835	1.00	27.46		A	C
ANISOU	1393	CA	ALA A 441	3496	3541	3397	3	43	15	A	C
ATOM	1395	CB	ALA A 441	14.459	-6.747	0.245	1.00	27.36		A	C
ANISOU	1395	CB	ALA A 441	3536	3457	3400	-28	-19	98	A	C
ATOM	1399	C	ALA A 441	14.295	-5.669	-2.041	1.00	27.59		A	C
ANISOU	1399	C	ALA A 441	3588	3474	3418	21	31	9	A	C
ATOM	1400	O	ALA A 441	14.622	-4.842	-2.894	1.00	27.73		A	O
ANISOU	1400	O	ALA A 441	3674	3678	3183	42	152	32	A	O
ATOM	1401	N	GLU A 442	13.211	-6.402	-2.169	1.00	28.14		A	N
ANISOU	1401	N	GLU A 442	3641	3590	3460	18	28	1	A	N
ATOM	1403	CA	GLU A 442	12.315	-6.144	-3.283	1.00	29.19		A	C
ANISOU	1403	CA	GLU A 442	3746	3741	3602	25	2	12	A	C
ATOM	1405	CB	GLU A 442	11.143	-7.127	-3.272	1.00	29.39		A	C
ANISOU	1405	CB	GLU A 442	3761	3759	3645	9	1	-19	A	C
ATOM	1408	CG	GLU A 442	10.232	-7.099	-2.043	1.00	30.59		A	C
ANISOU	1408	CG	GLU A 442	3900	3970	3752	23	27	40	A	C
ATOM	1411	CD	GLU A 442	10.615	-8.048	-0.890	1.00	31.18		A	C
ANISOU	1411	CD	GLU A 442	3920	4006	3921	-21	14	30	A	C
ATOM	1412	OE1	GLU A 442	11.806	-8.287	-0.605	1.00	28.47		A	O
ANISOU	1412	OE1	GLU A 442	3855	3761	3202	21	39	11	A	O
ATOM	1413	OE2	GLU A 442	9.686	-8.518	-0.200	1.00	31.93		A	O
ANISOU	1413	OE2	GLU A 442	4194	4085	3852	-88	70	84	A	O
ATOM	1414	C	GLU A 442	11.890	-4.659	-3.297	1.00	29.49		A	C
ANISOU	1414	C	GLU A 442	3814	3755	3633	32	-10	25	A	C
ATOM	1415	O	GLU A 442	11.675	-4.072	-4.365	1.00	30.02		A	O
ANISOU	1415	O	GLU A 442	3921	3905	3578	93	0	47	A	O

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ATOM	1416	N	SER	A	443	11.767	-4.063	-2.108	1.00	28.94		A	N
ANISOU	1416	N	SER	A	443	3774	3703	3518	32	5	31	A	N
ATOM	1418	CA	SER	A	443	11.585	-2.624	-1.934	1.00	29.65		A	C
ANISOU	1418	CA	SER	A	443	3806	3797	3661	38	2	9	A	C
ATOM	1420	CB	SER	A	443	10.137	-2.282	-1.555	1.00	30.34		A	C
ANISOU	1420	CB	SER	A	443	3887	3846	3794	49	-1	-13	A	C
ATOM	1423	OG	SER	A	443	9.182	-2.814	-2.469	1.00	32.78		A	O
ANISOU	1423	OG	SER	A	443	4082	4303	4067	65	-82	-40	A	O
ATOM	1425	C	SER	A	443	12.511	-2.204	-0.790	1.00	28.77		A	C
ANISOU	1425	C	SER	A	443	3779	3626	3524	43	30	-33	A	C
ATOM	1426	O	SER	A	443	13.058	-3.062	-0.102	1.00	27.90		A	O
ANISOU	1426	O	SER	A	443	3773	3553	3273	109	21	-94	A	O
ATOM	1427	N	TRP	A	444	12.729	-0.902	-0.603	1.00	28.54		A	N
ANISOU	1427	N	TRP	A	444	3742	3618	3482	-10	17	56	A	N
ATOM	1429	CA	TRP	A	444	13.448	-0.408	0.575	1.00	28.43		A	C
ANISOU	1429	CA	TRP	A	444	3678	3579	3545	18	45	29	A	C
ATOM	1431	CB	TRP	A	444	13.868	1.048	0.403	1.00	29.01		A	C
ANISOU	1431	CB	TRP	A	444	3753	3612	3656	-25	21	-8	A	C
ATOM	1434	CG	TRP	A	444	15.217	1.235	-0.227	1.00	31.09		A	C
ANISOU	1434	CG	TRP	A	444	3993	3851	3968	-19	93	16	A	C
ATOM	1435	CD1	TRP	A	444	15.472	1.561	-1.533	1.00	32.14		A	C
ANISOU	1435	CD1	TRP	A	444	4178	4021	4010	10	73	19	A	C
ATOM	1437	NE1	TRP	A	444	16.825	1.655	-1.735	1.00	33.31		A	N
ANISOU	1437	NE1	TRP	A	444	4253	4185	4217	-59	48	62	A	N
ATOM	1439	CE2	TRP	A	444	17.476	1.406	-0.557	1.00	33.68		A	C
ANISOU	1439	CE2	TRP	A	444	4300	4228	4267	-29	44	44	A	C
ATOM	1440	CD2	TRP	A	444	16.492	1.141	0.416	1.00	31.95		A	C
ANISOU	1440	CD2	TRP	A	444	4100	3929	4111	-6	54	-20	A	C
ATOM	1441	CE3	TRP	A	444	16.906	0.843	1.707	1.00	34.05		A	C
ANISOU	1441	CE3	TRP	A	444	4375	4237	4324	20	-15	-58	A	C
ATOM	1443	CZ3	TRP	A	444	18.249	0.835	1.996	1.00	35.56		A	C
ANISOU	1443	CZ3	TRP	A	444	4438	4509	4564	7	61	-22	A	C
ATOM	1445	CH2	TRP	A	444	19.206	1.102	1.011	1.00	35.88		A	C
ANISOU	1445	CH2	TRP	A	444	4578	4522	4530	-48	35	12	A	C
ATOM	1447	CZ2	TRP	A	444	18.840	1.394	-0.267	1.00	34.47		A	C
ANISOU	1447	CZ2	TRP	A	444	4372	4289	4436	-19	49	29	A	C
ATOM	1449	C	TRP	A	444	12.465	-0.544	1.749	1.00	27.01		A	C
ANISOU	1449	C	TRP	A	444	3511	3446	3305	44	35	51	A	C
ATOM	1450	O	TRP	A	444	11.267	-0.232	1.615	1.00	25.29		A	O
ANISOU	1450	O	TRP	A	444	3463	3276	2870	18	65	117	A	O
ATOM	1451	N	MET	A	445	12.972	-1.039	2.878	1.00	25.77		A	N
ANISOU	1451	N	MET	A	445	3335	3290	3163	54	67	-8	A	N
ATOM	1453	CA	MET	A	445	12.159	-1.310	4.056	1.00	24.66		A	C
ANISOU	1453	CA	MET	A	445	3191	3134	3044	-19	29	-9	A	C
ATOM	1455	CB	MET	A	445	12.028	-2.816	4.231	1.00	25.44		A	C
ANISOU	1455	CB	MET	A	445	3334	3199	3130	27	32	10	A	C
ATOM	1458	CG	MET	A	445	11.394	-3.544	3.058	1.00	25.85		A	C
ANISOU	1458	CG	MET	A	445	3387	3186	3247	-4	11	-13	A	C
ATOM	1461	SD	MET	A	445	11.420	-5.329	3.294	1.00	26.91		A	S
ANISOU	1461	SD	MET	A	445	3936	3156	3130	-209	164	-13	A	S
ATOM	1462	CE	MET	A	445	10.948	-5.936	1.671	1.00	29.23		A	C
ANISOU	1462	CE	MET	A	445	3861	3738	3507	40	30	-78	A	C
ATOM	1466	C	MET	A	445	12.806	-0.735	5.309	1.00	23.05		A	C
ANISOU	1466	C	MET	A	445	3010	2926	2819	22	72	0	A	C
ATOM	1467	O	MET	A	445	14.039	-0.788	5.482	1.00	22.63		A	O
ANISOU	1467	O	MET	A	445	3086	2993	2518	0	107	-78	A	O
ATOM	1468	N	LEU	A	446	11.949	-0.209	6.178	1.00	21.88		A	N
ANISOU	1468	N	LEU	A	446	2949	2674	2690	-43	75	9	A	N
ATOM	1470	CA	LEU	A	446	12.328	0.279	7.492	1.00	21.21		A	C
ANISOU	1470	CA	LEU	A	446	2801	2630	2624	-20	25	65	A	C
ATOM	1472	CB	LEU	A	446	11.794	1.692	7.682	1.00	21.93		A	C
ANISOU	1472	CB	LEU	A	446	2904	2661	2765	-34	97	38	A	C

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ATOM	1475	CG	LEU	A	446	12.024	2.312	9.047	1.00	24.60		A	C
ANISOU	1475	CG	LEU	A	446	3251	3070	3023	3	24	1	A	C
ATOM	1477	CD1	LEU	A	446	13.459	2.250	9.407	1.00	25.12		A	C
ANISOU	1477	CD1	LEU	A	446	3224	3085	3232	-42	28	-10	A	C
ATOM	1481	CD2	LEU	A	446	11.523	3.745	9.059	1.00	27.19		A	C
ANISOU	1481	CD2	LEU	A	446	3583	3238	3507	1	-4	-14	A	C
ATOM	1485	C	LEU	A	446	11.642	-0.656	8.493	1.00	19.97		A	C
ANISOU	1485	C	LEU	A	446	2672	2539	2375	7	64	21	A	C
ATOM	1486	O	LEU	A	446	10.417	-0.710	8.549	1.00	20.15		A	O
ANISOU	1486	O	LEU	A	446	2881	2498	2275	-54	206	78	A	O
ATOM	1487	N	VAL	A	447	12.450	-1.422	9.218	1.00	19.14		A	N
ANISOU	1487	N	VAL	A	447	2518	2485	2267	-33	115	2	A	N
ATOM	1489	CA	VAL	A	447	11.939	-2.453	10.119	1.00	18.69		A	C
ANISOU	1489	CA	VAL	A	447	2505	2375	2220	-27	56	15	A	C
ATOM	1491	CB	VAL	A	447	12.855	-3.710	10.057	1.00	18.72		A	C
ANISOU	1491	CB	VAL	A	447	2487	2367	2255	1	93	-3	A	C
ATOM	1493	CG1	VAL	A	447	12.338	-4.808	10.928	1.00	18.51		A	C
ANISOU	1493	CG1	VAL	A	447	2488	2407	2138	29	114	4	A	C
ATOM	1497	CG2	VAL	A	447	12.976	-4.236	8.616	1.00	19.67		A	C
ANISOU	1497	CG2	VAL	A	447	2643	2492	2337	-20	0	-65	A	C
ATOM	1501	C	VAL	A	447	11.935	-1.885	11.534	1.00	18.70		A	C
ANISOU	1501	C	VAL	A	447	2450	2419	2236	-49	74	-22	A	C
ATOM	1502	O	VAL	A	447	12.963	-1.429	12.015	1.00	18.95		A	O
ANISOU	1502	O	VAL	A	447	2488	2558	2151	-150	205	-49	A	O
ATOM	1503	N	MET	A	448	10.776	-1.926	12.184	1.00	17.94		A	N
ANISOU	1503	N	MET	A	448	2400	2271	2144	-57	58	-24	A	N
ATOM	1505	CA	MET	A	448	10.587	-1.308	13.499	1.00	18.19		A	C
ANISOU	1505	CA	MET	A	448	2420	2272	2220	-6	93	-25	A	C
ATOM	1507	CB	MET	A	448	9.645	-0.125	13.329	1.00	18.71		A	C
ANISOU	1507	CB	MET	A	448	2519	2391	2196	22	56	-33	A	C
ATOM	1510	CG	MET	A	448	10.240	0.961	12.463	1.00	21.84		A	C
ANISOU	1510	CG	MET	A	448	2956	2691	2650	-4	94	-40	A	C
ATOM	1513	SD	MET	A	448	8.998	2.102	11.951	1.00	24.05		A	S
ANISOU	1513	SD	MET	A	448	3556	2599	2982	83	172	76	A	S
ATOM	1514	CE	MET	A	448	8.206	1.186	10.633	1.00	25.39		A	C
ANISOU	1514	CE	MET	A	448	3283	3312	3052	-4	79	41	A	C
ATOM	1518	C	MET	A	448	9.977	-2.287	14.491	1.00	17.76		A	C
ANISOU	1518	C	MET	A	448	2351	2249	2146	4	50	-1	A	C
ATOM	1519	O	MET	A	448	9.438	-3.310	14.096	1.00	17.90		A	O
ANISOU	1519	O	MET	A	448	2483	2225	2092	55	157	59	A	O
ATOM	1520	N	GLU	A	449	9.997	-1.911	15.768	1.00	17.94		A	N
ANISOU	1520	N	GLU	A	449	2360	2249	2207	-30	66	20	A	N
ATOM	1522	CA	GLU	A	449	9.286	-2.649	16.781	1.00	18.53		A	C
ANISOU	1522	CA	GLU	A	449	2442	2276	2320	-34	29	19	A	C
ATOM	1524	CB	GLU	A	449	9.401	-1.963	18.135	1.00	19.17		A	C
ANISOU	1524	CB	GLU	A	449	2480	2515	2286	-89	63	97	A	C
ATOM	1527	CG	AGLU	A	449	10.802	-1.976	18.722	0.50	20.64		A	C
ANISOU	1527	CG	AGLU	A	449	2631	2657	2553	30	8	79	A	C
ATOM	1528	CG	BGLU	A	449	10.784	-1.799	18.659	0.50	19.99		A	C
ANISOU	1528	CG	BGLU	A	449	2605	2561	2427	-2	-5	50	A	C
ATOM	1533	CD	AGLU	A	449	10.949	-1.156	20.010	0.50	22.18		A	C
ANISOU	1533	CD	AGLU	A	449	2960	2738	2726	89	33	0	A	C
ATOM	1534	CD	BGLU	A	449	10.724	-1.449	20.112	0.50	20.45		A	C
ANISOU	1534	CD	BGLU	A	449	2804	2492	2471	-25	13	1	A	C
ATOM	1535	OE1AGLU	A	449	10.307	-0.082	20.148	0.50	19.92			A	O
ANISOU	1535	OE1AGLU	A	449	2717	2485	2364	111	-143	80		A	O
ATOM	1536	OE1BGLU	A	449	10.608	-0.227	20.448	0.50	19.03			A	O
ANISOU	1536	OE1BGLU	A	449	2781	2300	2148	22	-53	95		A	O
ATOM	1537	OE2AGLU	A	449	11.734	-1.579	20.902	0.50	23.91			A	O
ANISOU	1537	OE2AGLU	A	449	3007	3092	2985	67	-73	60		A	O
ATOM	1538	OE2BGLU	A	449	10.763	-2.425	20.895	0.50	19.94			A	O
ANISOU	1538	OE2BGLU	A	449	2705	2439	2432	-151	-46	45		A	O



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Figure 1A – 25

ATOM	1539	C	GLU	A	449	7.809	-2.634	16.419	1.00	17.83		A	C
ANISOU	1539	C	GLU	A	449	2334	2219	2221	-9	55	24	A	C
ATOM	1540	O	GLU	A	449	7.332	-1.716	15.763	1.00	17.74		A	O
ANISOU	1540	O	GLU	A	449	2362	2078	2299	-70	34	-71	A	O
ATOM	1541	N	MET	A	450	7.074	-3.634	16.900	1.00	17.47		A	N
ANISOU	1541	N	MET	A	450	2267	2167	2203	-24	69	38	A	N
ATOM	1543	CA	MET	A	450	5.648	-3.707	16.714	1.00	17.66		A	C
ANISOU	1543	CA	MET	A	450	2328	2158	2223	3	6	13	A	C
ATOM	1545	CB	MET	A	450	5.278	-5.141	16.340	1.00	18.22		A	C
ANISOU	1545	CB	MET	A	450	2350	2206	2366	-21	14	45	A	C
ATOM	1548	CG	AMET	A	450	4.842	-5.304	14.880	0.50	22.76		A	C
ANISOU	1548	CG	AMET	A	450	3129	2802	2714	21	39	-28	A	C
ATOM	1549	CG	BMET	A	450	3.918	-5.239	15.602	0.50	16.87		A	C
ANISOU	1549	CG	BMET	A	450	2157	1901	2349	-65	19	-135	A	C
ATOM	1554	SD	AMET	A	450	3.197	-5.523	14.511	0.50	29.38		A	S
ANISOU	1554	SD	AMET	A	450	3576	3967	3621	101	-140	89	A	S
ATOM	1555	SD	BMET	A	450	3.222	-6.953	15.521	0.50	17.40		A	S
ANISOU	1555	SD	BMET	A	450	2491	1787	2331	-229	-36	-212	A	S
ATOM	1556	CE	AMET	A	450	2.530	-4.531	15.611	0.50	30.46		A	C
ANISOU	1556	CE	AMET	A	450	3906	3868	3797	-21	-9	-18	A	C
ATOM	1557	CE	BMET	A	450	4.319	-7.500	14.180	0.50	19.30		A	C
ANISOU	1557	CE	BMET	A	450	2405	2468	2458	-24	48	-21	A	C
ATOM	1564	C	MET	A	450	4.887	-3.271	17.980	1.00	16.85		A	C
ANISOU	1564	C	MET	A	450	2157	2095	2151	-57	22	65	A	C
ATOM	1565	O	MET	A	450	5.279	-3.607	19.089	1.00	18.37		A	O
ANISOU	1565	O	MET	A	450	2410	2349	2218	38	51	111	A	O
ATOM	1566	N	ALA	A	451	3.813	-2.518	17.800	1.00	16.82		A	N
ANISOU	1566	N	ALA	A	451	2238	2029	2123	-18	24	73	A	N
ATOM	1568	CA	ALA	A	451	2.905	-2.116	18.870	1.00	16.04		A	C
ANISOU	1568	CA	ALA	A	451	2117	1883	2093	-30	27	16	A	C
ATOM	1570	CB	ALA	A	451	2.986	-0.594	19.041	1.00	16.33		A	C
ANISOU	1570	CB	ALA	A	451	2206	1860	2137	44	23	-39	A	C
ATOM	1574	C	ALA	A	451	1.518	-2.549	18.389	1.00	17.25		A	C
ANISOU	1574	C	ALA	A	451	2249	2073	2230	12	2	-55	A	C
ATOM	1575	O	ALA	A	451	0.739	-1.739	17.854	1.00	18.62		A	O
ANISOU	1575	O	ALA	A	451	2302	2291	2482	-154	-35	16	A	O
ATOM	1576	N	GLU	A	452	1.192	-3.832	18.566	1.00	18.68		A	N
ANISOU	1576	N	GLU	A	452	2403	2248	2444	-24	-4	5	A	N
ATOM	1578	CA	GLU	A	452	0.070	-4.392	17.797	1.00	19.74		A	C
ANISOU	1578	CA	GLU	A	452	2547	2385	2565	-24	-53	-31	A	C
ATOM	1580	CB	GLU	A	452	0.167	-5.912	17.719	1.00	20.87		A	C
ANISOU	1580	CB	GLU	A	452	2719	2459	2751	12	-81	0	A	C
ATOM	1583	CG	GLU	A	452	-0.689	-6.488	16.614	1.00	21.75		A	C
ANISOU	1583	CG	GLU	A	452	2826	2615	2820	-9	-78	-29	A	C
ATOM	1586	CD	GLU	A	452	-0.619	-7.999	16.548	1.00	22.32		A	C
ANISOU	1586	CD	GLU	A	452	2957	2632	2890	35	-57	18	A	C
ATOM	1587	OE1	GLU	A	452	-0.152	-8.641	17.531	1.00	19.29		A	O
ANISOU	1587	OE1	GLU	A	452	2538	2358	2434	-152	-83	-104	A	O
ATOM	1588	OE2	GLU	A	452	-1.019	-8.507	15.485	1.00	23.06		A	O
ANISOU	1588	OE2	GLU	A	452	3049	2688	3025	-60	-155	-68	A	O
ATOM	1589	C	GLU	A	452	-1.320	-4.000	18.185	1.00	19.76		A	C
ANISOU	1589	C	GLU	A	452	2546	2387	2574	-76	-63	-23	A	C
ATOM	1590	O	GLU	A	452	-2.279	-4.240	17.429	1.00	20.88		A	O
ANISOU	1590	O	GLU	A	452	2639	2570	2722	-170	-103	-35	A	O
ATOM	1591	N	LEU	A	453	-1.462	-3.352	19.326	1.00	19.64		A	N
ANISOU	1591	N	LEU	A	453	2458	2360	2643	-79	-31	-13	A	N
ATOM	1593	CA	LEU	A	453	-2.754	-2.949	19.739	1.00	20.28		A	C
ANISOU	1593	CA	LEU	A	453	2563	2501	2640	-17	-34	-18	A	C
ATOM	1595	CB	LEU	A	453	-2.774	-2.735	21.227	1.00	21.23		A	C
ANISOU	1595	CB	LEU	A	453	2682	2629	2755	52	-17	-96	A	C
ATOM	1598	CG	LEU	A	453	-3.256	-3.907	22.038	1.00	24.24		A	C
ANISOU	1598	CG	LEU	A	453	3021	3133	3056	24	25	-23	A	C

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Figure 1A – 26

ATOM	1600	CD1	LEU	A	453	-2.407	-5.116	21.811	1.00	25.74		A	C
ANISOU	1600	CD1	LEU	A	453	3259	3229	3290	35	40	45	A	C
ATOM	1604	CD2	LEU	A	453	-3.282	-3.525	23.495	1.00	25.46		A	C
ANISOU	1604	CD2	LEU	A	453	3286	3259	3127	-9	-13	35	A	C
ATOM	1608	C	LEU	A	453	-3.160	-1.704	18.962	1.00	20.26		A	C
ANISOU	1608	C	LEU	A	453	2589	2478	2629	6	30	-50	A	C
ATOM	1609	O	LEU	A	453	-4.322	-1.323	18.979	1.00	20.72		A	O
ANISOU	1609	O	LEU	A	453	2614	2447	2811	110	-142	-127	A	O
ATOM	1610	N	GLY	A	454	-2.215	-1.097	18.260	1.00	19.38		A	N
ANISOU	1610	N	GLY	A	454	2519	2320	2523	-35	-47	-67	A	N
ATOM	1612	CA	GLY	A	454	-2.576	-0.025	17.351	1.00	18.80		A	C
ANISOU	1612	CA	GLY	A	454	2456	2282	2404	-12	14	-15	A	C
ATOM	1615	C	GLY	A	454	-2.738	1.385	17.869	1.00	18.47		A	C
ANISOU	1615	C	GLY	A	454	2440	2215	2361	-44	-14	-8	A	C
ATOM	1616	O	GLY	A	454	-2.458	1.697	19.029	1.00	17.54		A	O
ANISOU	1616	O	GLY	A	454	2401	2026	2237	27	-22	91	A	O
ATOM	1617	N	PRO	A	455	-3.204	2.242	16.976	1.00	18.63		A	N
ANISOU	1617	N	PRO	A	455	2428	2225	2425	-9	-70	-11	A	N
ATOM	1618	CA	PRO	A	455	-3.309	3.676	17.272	1.00	18.56		A	C
ANISOU	1618	CA	PRO	A	455	2364	2257	2429	-31	-64	-34	A	C
ATOM	1620	CB	PRO	A	455	-3.906	4.264	15.990	1.00	18.51		A	C
ANISOU	1620	CB	PRO	A	455	2340	2254	2439	-45	-36	11	A	C
ATOM	1623	CG	PRO	A	455	-3.765	3.261	14.969	1.00	20.51		A	C
ANISOU	1623	CG	PRO	A	455	2703	2573	2515	59	-106	54	A	C
ATOM	1626	CD	PRO	A	455	-3.708	1.936	15.635	1.00	20.13		A	C
ANISOU	1626	CD	PRO	A	455	2724	2365	2559	-17	-24	-47	A	C
ATOM	1629	C	PRO	A	455	-4.200	3.974	18.462	1.00	18.20		A	C
ANISOU	1629	C	PRO	A	455	2287	2253	2371	-72	-79	21	A	C
ATOM	1630	O	PRO	A	455	-5.268	3.388	18.653	1.00	19.26		A	O
ANISOU	1630	O	PRO	A	455	2283	2321	2711	-141	-81	13	A	O
ATOM	1631	N	LEU	A	456	-3.767	4.945	19.250	1.00	17.29		A	N
ANISOU	1631	N	LEU	A	456	2252	2103	2215	-65	-100	-34	A	N
ATOM	1633	CA	LEU	A	456	-4.470	5.366	20.453	1.00	17.34		A	C
ANISOU	1633	CA	LEU	A	456	2124	2159	2304	-33	-63	33	A	C
ATOM	1635	CB	LEU	A	456	-3.647	6.464	21.136	1.00	17.47		A	C
ANISOU	1635	CB	LEU	A	456	2162	2142	2332	-14	-117	-31	A	C
ATOM	1638	CG	LEU	A	456	-4.229	7.063	22.410	1.00	18.38		A	C
ANISOU	1638	CG	LEU	A	456	2295	2336	2350	-43	-29	42	A	C
ATOM	1640	CD1	LEU	A	456	-4.316	6.036	23.530	1.00	19.00		A	C
ANISOU	1640	CD1	LEU	A	456	2355	2447	2415	82	49	94	A	C
ATOM	1644	CD2	LEU	A	456	-3.389	8.253	22.844	1.00	18.57		A	C
ANISOU	1644	CD2	LEU	A	456	2339	2176	2540	132	-16	-17	A	C
ATOM	1648	C	LEU	A	456	-5.854	5.898	20.163	1.00	17.94		A	C
ANISOU	1648	C	LEU	A	456	2196	2231	2390	19	20	-12	A	C
ATOM	1649	O	LEU	A	456	-6.764	5.661	20.935	1.00	19.06		A	O
ANISOU	1649	O	LEU	A	456	2286	2395	2557	-54	4	117	A	O
ATOM	1650	N	ASN	A	457	-6.010	6.620	19.055	1.00	18.51		A	N
ANISOU	1650	N	ASN	A	457	2199	2345	2486	-10	-70	11	A	N
ATOM	1652	CA	ASN	A	457	-7.323	7.199	18.770	1.00	19.51		A	C
ANISOU	1652	CA	ASN	A	457	2386	2426	2602	-19	-79	59	A	C
ATOM	1654	CB	ASN	A	457	-7.278	8.304	17.690	1.00	19.25		A	C
ANISOU	1654	CB	ASN	A	457	2304	2397	2613	-45	-195	66	A	C
ATOM	1657	CG	ASN	A	457	-6.701	7.861	16.350	1.00	21.01		A	C
ANISOU	1657	CG	ASN	A	457	2518	2695	2768	-48	-98	111	A	C
ATOM	1658	OD1	ASN	A	457	-5.994	6.850	16.225	1.00	21.25		A	O
ANISOU	1658	OD1	ASN	A	457	2575	2649	2849	-132	-188	-3	A	O
ATOM	1659	ND2	ASN	A	457	-6.984	8.681	15.304	1.00	22.43		A	N
ANISOU	1659	ND2	ASN	A	457	2621	3015	2883	-27	-266	155	A	N
ATOM	1662	C	ASN	A	457	-8.349	6.116	18.480	1.00	20.09		A	C
ANISOU	1662	C	ASN	A	457	2411	2554	2669	-25	-93	76	A	C
ATOM	1663	O	ASN	A	457	-9.443	6.137	19.048	1.00	22.01		A	O
ANISOU	1663	O	ASN	A	457	2626	2723	3013	-169	-23	94	A	O

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Figure 1A – 27

ATOM	1664	N	LYS	A	458	-7.965	5.170	17.651	1.00	20.79		A	N
ANISOU	1664	N	LYS	A	458	2513	2598	2789	-107	-126	47	A	N
ATOM	1666	CA	LYS	A	458	-8.839	4.040	17.321	1.00	22.12		A	C
ANISOU	1666	CA	LYS	A	458	2717	2748	2936	-76	-78	5	A	C
ATOM	1668	CB	LYS	A	458	-8.179	3.148	16.288	1.00	22.84		A	C
ANISOU	1668	CB	LYS	A	458	2842	2823	3011	-104	-29	18	A	C
ATOM	1671	CG	ALYS	A	458	-9.138	2.335	15.413	0.50	23.32		A	C
ANISOU	1671	CG	ALYS	A	458	2900	2932	3028	-90	-24	11	A	C
ATOM	1672	CG	BLYS	A	458	-8.714	3.343	14.857	0.50	25.89		A	C
ANISOU	1672	CG	BLYS	A	458	3293	3256	3286	-15	-55	64	A	C
ATOM	1677	CD	ALYS	A	458	-8.439	1.573	14.323	0.50	24.44		A	C
ANISOU	1677	CD	ALYS	A	458	3062	3046	3178	13	0	-42	A	C
ATOM	1678	CD	BLYS	A	458	-7.767	2.815	13.758	0.50	28.46		A	C
ANISOU	1678	CD	BLYS	A	458	3586	3624	3602	7	40	-30	A	C
ATOM	1683	CE	ALYS	A	458	-9.144	0.252	14.042	0.50	26.12		A	C
ANISOU	1683	CE	ALYS	A	458	3256	3269	3397	-62	-19	-39	A	C
ATOM	1684	CE	BLYS	A	458	-7.788	3.686	12.496	0.50	30.24		A	C
ANISOU	1684	CE	BLYS	A	458	3888	3799	3800	19	-19	34	A	C
ATOM	1689	NZ	ALYS	A	458	-8.568	-0.456	12.864	0.50	28.11		A	N
ANISOU	1689	NZ	ALYS	A	458	3536	3623	3519	38	1	-75	A	N
ATOM	1690	NZ	BLYS	A	458	-7.895	2.876	11.251	0.50	32.09		A	N
ANISOU	1690	NZ	BLYS	A	458	4111	4103	3975	32	1	-62	A	N
ATOM	1697	C	LYS	A	458	-9.129	3.233	18.566	1.00	22.63		A	C
ANISOU	1697	C	LYS	A	458	2784	2845	2970	-70	-64	19	A	C
ATOM	1698	O	LYS	A	458	-10.269	2.791	18.807	1.00	23.35		A	O
ANISOU	1698	O	LYS	A	458	2759	2975	3136	-124	-122	130	A	O
ATOM	1699	N	TYR	A	459	-8.110	3.038	19.401	1.00	22.41		A	N
ANISOU	1699	N	TYR	A	459	2759	2770	2983	-69	-93	35	A	N
ATOM	1701	CA	TYR	A	459	-8.297	2.203	20.570	1.00	23.28		A	C
ANISOU	1701	CA	TYR	A	459	2888	2922	3034	-52	-56	18	A	C
ATOM	1703	CB	TYR	A	459	-6.964	2.012	21.308	1.00	22.59		A	C
ANISOU	1703	CB	TYR	A	459	2774	2771	3037	-88	-50	17	A	C
ATOM	1706	CG	TYR	A	459	-7.062	1.076	22.480	1.00	23.87		A	C
ANISOU	1706	CG	TYR	A	459	2850	3072	3147	27	-110	70	A	C
ATOM	1707	CD1	TYR	A	459	-6.915	-0.283	22.298	1.00	26.01		A	C
ANISOU	1707	CD1	TYR	A	459	3270	3241	3370	-67	-2	-7	A	C
ATOM	1709	CE1	TYR	A	459	-7.006	-1.153	23.355	1.00	26.91		A	C
ANISOU	1709	CE1	TYR	A	459	3414	3367	3442	0	-43	144	A	C
ATOM	1711	CZ	TYR	A	459	-7.220	-0.649	24.627	1.00	28.36		A	C
ANISOU	1711	CZ	TYR	A	459	3518	3635	3621	-20	82	35	A	C
ATOM	1712	OH	TYR	A	459	-7.294	-1.518	25.702	1.00	34.02		A	O
ANISOU	1712	OH	TYR	A	459	4348	4360	4215	-5	2	337	A	O
ATOM	1714	CE2	TYR	A	459	-7.359	0.685	24.831	1.00	27.50		A	C
ANISOU	1714	CE2	TYR	A	459	3425	3619	3402	14	56	104	A	C
ATOM	1716	CD2	TYR	A	459	-7.270	1.549	23.747	1.00	24.89		A	C
ANISOU	1716	CD2	TYR	A	459	3057	3175	3225	56	-7	111	A	C
ATOM	1718	C	TYR	A	459	-9.348	2.798	21.490	1.00	23.23		A	C
ANISOU	1718	C	TYR	A	459	2900	2867	3058	-56	-17	30	A	C
ATOM	1719	O	TYR	A	459	-10.227	2.094	21.990	1.00	24.22		A	O
ANISOU	1719	O	TYR	A	459	2960	3008	3232	-49	15	128	A	O
ATOM	1720	N	LEU	A	460	-9.303	4.115	21.668	1.00	22.25		A	N
ANISOU	1720	N	LEU	A	460	2744	2688	3019	-65	-4	37	A	N
ATOM	1722	CA	LEU	A	460	-10.220	4.793	22.564	1.00	23.14		A	C
ANISOU	1722	CA	LEU	A	460	2919	2828	3043	-83	-2	23	A	C
ATOM	1724	CB	LEU	A	460	-9.637	6.146	22.948	1.00	22.42		A	C
ANISOU	1724	CB	LEU	A	460	2848	2679	2991	-68	-2	53	A	C
ATOM	1727	CG	LEU	A	460	-8.394	5.989	23.829	1.00	21.30		A	C
ANISOU	1727	CG	LEU	A	460	2685	2534	2871	-129	19	-4	A	C
ATOM	1729	CD1	LEU	A	460	-7.737	7.355	24.113	1.00	21.81		A	C
ANISOU	1729	CD1	LEU	A	460	2777	2643	2867	-106	60	-150	A	C
ATOM	1733	CD2	LEU	A	460	-8.716	5.312	25.144	1.00	23.60		A	C
ANISOU	1733	CD2	LEU	A	460	3068	2857	3041	-58	23	45	A	C

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Figure 1A – 28

ATOM	1737	C	LEU	A	460	-11.639	4.925	21.959	1.00	24.48		A	C
ANISOU	1737	C	LEU	A	460	2990	3054	3256	1	0	41	A	C
ATOM	1738	O	LEU	A	460	-12.635	5.022	22.714	1.00	25.47		A	O
ANISOU	1738	O	LEU	A	460	3014	3286	3375	11	-28	113	A	O
ATOM	1739	N	GLN	A	461	-11.733	4.922	20.634	1.00	26.07		A	N
ANISOU	1739	N	GLN	A	461	3218	3263	3423	-45	1	24	A	N
ATOM	1741	CA	GLN	A	461	-13.031	4.973	19.958	1.00	28.41		A	C
ANISOU	1741	CA	GLN	A	461	3517	3565	3711	-19	-17	8	A	C
ATOM	1743	CB	GLN	A	461	-12.889	5.057	18.444	1.00	29.38		A	C
ANISOU	1743	CB	GLN	A	461	3639	3730	3794	-25	-27	10	A	C
ATOM	1746	CG	AGLN	A	461	-14.193	5.586	17.715	0.50	30.36		A	C
ANISOU	1746	CG	AGLN	A	461	3754	3878	3902	-11	-44	-26	A	C
ATOM	1747	CG	BGLN	A	461	-13.050	6.420	17.787	0.50	31.57		A	C
ANISOU	1747	CG	BGLN	A	461	4048	3889	4054	0	-9	13	A	C
ATOM	1752	CD	AGLN	A	461	-14.169	6.982	17.148	0.50	32.39		A	C
ANISOU	1752	CD	AGLN	A	461	4079	4059	4166	30	-14	51	A	C
ATOM	1753	CD	BGLN	A	461	-12.259	6.513	16.475	0.50	34.06		A	C
ANISOU	1753	CD	BGLN	A	461	4335	4352	4251	-5	40	33	A	C
ATOM	1754	OE1	AGLN	A	461	-14.592	7.182	16.005	0.50	34.52		A	O
ANISOU	1754	OE1	AGLN	A	461	4384	4469	4263	-48	-21	-31	A	O
ATOM	1755	OE1	BGLN	A	461	-11.488	7.460	16.260	0.50	35.44		A	O
ANISOU	1755	OE1	BGLN	A	461	4524	4472	4467	-62	-74	-60	A	O
ATOM	1756	NE2	AGLN	A	461	-13.743	7.957	17.943	0.50	33.91		A	N
ANISOU	1756	NE2	AGLN	A	461	4289	4268	4325	-2	-55	-62	A	N
ATOM	1757	NE2	BGLN	A	461	-12.438	5.523	15.607	0.50	35.39		A	N
ANISOU	1757	NE2	BGLN	A	461	4587	4398	4461	21	17	-27	A	N
ATOM	1762	C	GLN	A	461	-13.757	3.662	20.203	1.00	29.52		A	C
ANISOU	1762	C	GLN	A	461	3652	3681	3882	-70	32	9	A	C
ATOM	1763	O	GLN	A	461	-14.953	3.639	20.520	1.00	30.33		A	O
ANISOU	1763	O	GLN	A	461	3673	3749	4101	-46	24	-1	A	O
ATOM	1764	N	GLN	A	462	-13.030	2.576	19.964	1.00	30.26		A	N
ANISOU	1764	N	GLN	A	462	3747	3760	3988	-68	21	14	A	N
ATOM	1766	CA	GLN	A	462	-13.567	1.214	20.105	1.00	31.44		A	C
ANISOU	1766	CA	GLN	A	462	3943	3915	4086	-87	-7	9	A	C
ATOM	1768	CB	GLN	A	462	-12.689	0.223	19.351	1.00	31.77		A	C
ANISOU	1768	CB	GLN	A	462	3944	3942	4182	-102	-5	0	A	C
ATOM	1771	CG	GLN	A	462	-12.530	0.545	17.898	1.00	34.48		A	C
ANISOU	1771	CG	GLN	A	462	4397	4341	4361	-84	-45	28	A	C
ATOM	1774	CD	GLN	A	462	-11.538	-0.360	17.197	1.00	38.63		A	C
ANISOU	1774	CD	GLN	A	462	4868	4839	4969	31	63	-34	A	C
ATOM	1775	OE1	GLN	A	462	-10.725	-1.028	17.837	1.00	41.57		A	O
ANISOU	1775	OE1	GLN	A	462	5072	5260	5461	48	-85	38	A	O
ATOM	1776	NE2	GLN	A	462	-11.605	-0.385	15.880	1.00	41.84		A	N
ANISOU	1776	NE2	GLN	A	462	5372	5387	5138	-3	81	-53	A	N
ATOM	1779	C	GLN	A	462	-13.708	0.721	21.527	1.00	31.87		A	C
ANISOU	1779	C	GLN	A	462	3987	3995	4124	-75	-7	29	A	C
ATOM	1780	O	GLN	A	462	-14.549	-0.134	21.794	1.00	32.64		A	O
ANISOU	1780	O	GLN	A	462	4064	4082	4256	-179	26	102	A	O
ATOM	1781	N	ASN	A	463	-12.862	1.207	22.426	1.00	32.02		A	N
ANISOU	1781	N	ASN	A	463	3991	4024	4150	-48	-4	36	A	N
ATOM	1783	CA	ASN	A	463	-12.888	0.801	23.820	1.00	32.54		A	C
ANISOU	1783	CA	ASN	A	463	4048	4128	4187	-48	-23	21	A	C
ATOM	1785	CB	ASN	A	463	-11.494	0.338	24.249	1.00	32.46		A	C
ANISOU	1785	CB	ASN	A	463	4084	4068	4180	-14	-19	55	A	C
ATOM	1788	CG	ASN	A	463	-11.059	-0.923	23.547	1.00	32.79		A	C
ANISOU	1788	CG	ASN	A	463	4085	4126	4248	-36	37	60	A	C
ATOM	1789	OD1	ASN	A	463	-11.402	-2.047	23.971	1.00	33.99		A	O
ANISOU	1789	OD1	ASN	A	463	4201	4100	4613	-141	56	115	A	O
ATOM	1790	ND2	ASN	A	463	-10.305	-0.769	22.464	1.00	31.21		A	N
ANISOU	1790	ND2	ASN	A	463	4129	3714	4016	-91	-68	176	A	N
ATOM	1793	C	ASN	A	463	-13.320	1.985	24.661	1.00	33.31		A	C
ANISOU	1793	C	ASN	A	463	4171	4190	4293	0	-25	14	A	C

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ATOM	1794	O	ASN	A	463	-12.499	2.620	25.321	1.00	32.78		A	O
ANISOU	1794	O	ASN	A	463	3971	4182	4301	32	-94	34	A	O
ATOM	1795	N	ARG	A	464	-14.619	2.276	24.668	1.00	34.02		A	N
ANISOU	1795	N	ARG	A	464	4199	4338	4387	-42	-43	21	A	N
ATOM	1797	CA	ARG	A	464	-15.120	3.477	25.327	1.00	35.47		A	C
ANISOU	1797	CA	ARG	A	464	4449	4491	4535	-8	-1	2	A	C
ATOM	1799	CB	ARG	A	464	-16.493	3.818	24.765	1.00	35.95		A	C
ANISOU	1799	CB	ARG	A	464	4470	4540	4649	-24	-19	-21	A	C
ATOM	1802	CG	ARG	A	464	-16.470	4.121	23.284	1.00	38.63		A	C
ANISOU	1802	CG	ARG	A	464	4897	4948	4830	-34	31	-23	A	C
ATOM	1805	CD	ARG	A	464	-17.523	5.130	22.862	1.00	42.51		A	C
ANISOU	1805	CD	ARG	A	464	5334	5390	5425	73	-61	9	A	C
ATOM	1808	NE	ARG	A	464	-17.201	5.761	21.588	1.00	45.14		A	N
ANISOU	1808	NE	ARG	A	464	5719	5768	5664	-74	12	21	A	N
ATOM	1810	CZ	ARG	A	464	-17.798	6.843	21.138	1.00	47.29		A	C
ANISOU	1810	CZ	ARG	A	464	5965	5958	6044	14	-52	34	A	C
ATOM	1811	NH1	ARG	A	464	-18.753	7.429	21.859	1.00	48.10		A	N
ANISOU	1811	NH1	ARG	A	464	6121	6088	6064	-1	30	-19	A	N
ATOM	1814	NH2	ARG	A	464	-17.451	7.347	19.964	1.00	48.99		A	N
ANISOU	1814	NH2	ARG	A	464	6131	6324	6156	-37	24	0	A	N
ATOM	1817	C	ARG	A	464	-15.200	3.434	26.845	1.00	35.57		A	C
ANISOU	1817	C	ARG	A	464	4435	4508	4572	-26	7	2	A	C
ATOM	1818	O	ARG	A	464	-15.576	4.424	27.487	1.00	36.12		A	O
ANISOU	1818	O	ARG	A	464	4514	4520	4687	-29	45	24	A	O
ATOM	1819	N	HIS	A	465	-14.823	2.306	27.429	1.00	35.63		A	N
ANISOU	1819	N	HIS	A	465	4461	4522	4553	-24	15	20	A	N
ATOM	1821	CA	HIS	A	465	-14.930	2.132	28.867	1.00	35.56		A	C
ANISOU	1821	CA	HIS	A	465	4445	4521	4544	-20	2	14	A	C
ATOM	1823	CB	HIS	A	465	-15.667	0.828	29.148	1.00	36.88		A	C
ANISOU	1823	CB	HIS	A	465	4671	4627	4713	-39	17	31	A	C
ATOM	1826	CG	HIS	A	465	-17.100	0.874	28.717	1.00	40.12		A	C
ANISOU	1826	CG	HIS	A	465	4927	5160	5156	-23	-38	45	A	C
ATOM	1827	ND1	HIS	A	465	-17.885	1.993	28.899	1.00	43.19		A	N
ANISOU	1827	ND1	HIS	A	465	5428	5389	5593	50	-42	-31	A	N
ATOM	1829	CE1	HIS	A	465	-19.091	1.771	28.407	1.00	44.24		A	C
ANISOU	1829	CE1	HIS	A	465	5505	5582	5722	-24	-24	-11	A	C
ATOM	1831	NE2	HIS	A	465	-19.117	0.547	27.910	1.00	44.48		A	N
ANISOU	1831	NE2	HIS	A	465	5547	5595	5759	38	-39	-41	A	N
ATOM	1833	CD2	HIS	A	465	-17.879	-0.032	28.080	1.00	42.64		A	C
ANISOU	1833	CD2	HIS	A	465	5385	5365	5450	-56	-54	-63	A	C
ATOM	1835	C	HIS	A	465	-13.580	2.193	29.549	1.00	33.97		A	C
ANISOU	1835	C	HIS	A	465	4266	4315	4326	-44	52	31	A	C
ATOM	1836	O	HIS	A	465	-13.448	1.971	30.747	1.00	33.37		A	O
ANISOU	1836	O	HIS	A	465	4097	4256	4325	-104	26	123	A	O
ATOM	1837	N	VAL	A	466	-12.566	2.519	28.770	1.00	32.31		A	N
ANISOU	1837	N	VAL	A	466	4035	4086	4154	-31	15	55	A	N
ATOM	1839	CA	VAL	A	466	-11.255	2.730	29.332	1.00	30.98		A	C
ANISOU	1839	CA	VAL	A	466	3898	3923	3951	-23	14	42	A	C
ATOM	1841	CB	VAL	A	466	-10.281	3.087	28.236	1.00	30.88		A	C
ANISOU	1841	CB	VAL	A	466	3868	3937	3926	-16	35	25	A	C
ATOM	1843	CG1	VAL	A	466	-8.968	3.571	28.818	1.00	31.43		A	C
ANISOU	1843	CG1	VAL	A	466	3953	4016	3970	-32	9	-9	A	C
ATOM	1847	CG2	VAL	A	466	-10.054	1.882	27.346	1.00	31.20		A	C
ANISOU	1847	CG2	VAL	A	466	3889	3948	4017	-71	22	3	A	C
ATOM	1851	C	VAL	A	466	-11.350	3.853	30.354	1.00	29.75		A	C
ANISOU	1851	C	VAL	A	466	3692	3774	3836	-46	38	89	A	C
ATOM	1852	O	VAL	A	466	-11.868	4.922	30.083	1.00	30.10		A	O
ANISOU	1852	O	VAL	A	466	3589	3830	4018	-21	38	146	A	O
ATOM	1853	N	LYS	A	467	-10.858	3.599	31.548	1.00	28.41		A	N
ANISOU	1853	N	LYS	A	467	3530	3587	3676	-67	61	52	A	N
ATOM	1855	CA	LYS	A	467	-10.991	4.554	32.622	1.00	27.54		A	C
ANISOU	1855	CA	LYS	A	467	3453	3435	3574	-48	45	49	A	C

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ATOM	1857	CB	LYS A 467	-10.688	3.874	33.944	1.00	27.96		A	C
ANISOU	1857	CB	LYS A 467	3495	3532	3597	-6	40	31	A	C
ATOM	1860	CG	LYS A 467	-11.734	2.815	34.338	1.00	30.41		A	C
ANISOU	1860	CG	LYS A 467	3873	3748	3934	-101	19	58	A	C
ATOM	1863	CD	LYS A 467	-13.016	3.374	34.938	0.00	39.76		A	C
ANISOU	1863	CD	LYS A 467	5035	5035	5035	0	0	0	A	C
ATOM	1866	CE	LYS A 467	-13.934	2.287	35.507	0.00	43.32		A	C
ANISOU	1866	CE	LYS A 467	5486	5486	5486	0	0	0	A	C
ATOM	1869	NZ	LYS A 467	-14.511	1.505	34.414	0.00	45.62		A	N
ANISOU	1869	NZ	LYS A 467	5777	5777	5777	0	0	0	A	N
ATOM	1873	C	LYS A 467	-10.082	5.761	32.442	1.00	26.44		A	C
ANISOU	1873	C	LYS A 467	3346	3277	3419	-12	86	21	A	C
ATOM	1874	O	LYS A 467	-9.048	5.682	31.780	1.00	23.03		A	O
ANISOU	1874	O	LYS A 467	3137	2656	2957	48	220	124	A	O
ATOM	1875	N	ASP A 468	-10.474	6.869	33.061	1.00	25.65		A	N
ANISOU	1875	N	ASP A 468	3221	3229	3295	26	122	11	A	N
ATOM	1877	CA	ASP A 468	-9.674	8.075	33.030	1.00	25.70		A	C
ANISOU	1877	CA	ASP A 468	3269	3229	3264	23	66	43	A	C
ATOM	1879	CB	ASP A 468	-10.260	9.108	33.968	1.00	27.22		A	C
ANISOU	1879	CB	ASP A 468	3470	3413	3457	43	58	-9	A	C
ATOM	1882	CG	ASP A 468	-11.470	9.787	33.393	1.00	30.82		A	C
ANISOU	1882	CG	ASP A 468	3801	3928	3980	99	-67	80	A	C
ATOM	1883	OD1	ASP A 468	-11.713	9.627	32.182	1.00	33.83		A	O
ANISOU	1883	OD1	ASP A 468	4237	4304	4310	151	23	-38	A	O
ATOM	1884	OD2	ASP A 468	-12.232	10.497	34.093	1.00	35.62		A	O
ANISOU	1884	OD2	ASP A 468	4337	4553	4643	222	111	-117	A	O
ATOM	1885	C	ASP A 468	-8.246	7.801	33.464	1.00	24.30		A	C
ANISOU	1885	C	ASP A 468	3138	3058	3035	9	65	69	A	C
ATOM	1886	O	ASP A 468	-7.292	8.308	32.873	1.00	23.09		A	O
ANISOU	1886	O	ASP A 468	2915	2825	3031	68	120	144	A	O
ATOM	1887	N	LYS A 469	-8.086	7.010	34.519	1.00	23.35		A	N
ANISOU	1887	N	LYS A 469	3005	2897	2967	25	87	117	A	N
ATOM	1889	CA	LYS A 469	-6.765	6.721	35.032	1.00	22.70		A	C
ANISOU	1889	CA	LYS A 469	2924	2858	2841	-11	105	96	A	C
ATOM	1891	CB	LYS A 469	-6.850	5.707	36.172	1.00	23.68		A	C
ANISOU	1891	CB	LYS A 469	3088	3057	2850	-8	127	114	A	C
ATOM	1894	CG	LYS A 469	-5.548	5.359	36.798	1.00	27.91		A	C
ANISOU	1894	CG	LYS A 469	3396	3736	3470	20	43	39	A	C
ATOM	1897	CD	LYS A 469	-5.578	3.994	37.540	1.00	33.21		A	C
ANISOU	1897	CD	LYS A 469	4321	4096	4198	31	3	95	A	C
ATOM	1900	CE	LYS A 469	-6.951	3.394	37.699	1.00	35.47		A	C
ANISOU	1900	CE	LYS A 469	4396	4635	4446	-22	34	-1	A	C
ATOM	1903	NZ	LYS A 469	-6.920	2.103	38.448	1.00	37.92		A	N
ANISOU	1903	NZ	LYS A 469	4775	4745	4885	18	4	46	A	N
ATOM	1907	C	LYS A 469	-5.872	6.120	33.954	1.00	20.68		A	C
ANISOU	1907	C	LYS A 469	2737	2546	2573	27	37	89	A	C
ATOM	1908	O	LYS A 469	-4.697	6.436	33.900	1.00	19.58		A	O
ANISOU	1908	O	LYS A 469	2690	2270	2479	46	78	142	A	O
ATOM	1909	N	ASN A 470	-6.433	5.249	33.122	1.00	19.68		A	N
ANISOU	1909	N	ASN A 470	2550	2451	2476	0	85	158	A	N
ATOM	1911	CA	ASN A 470	-5.698	4.525	32.097	1.00	18.53		A	C
ANISOU	1911	CA	ASN A 470	2359	2369	2311	13	70	159	A	C
ATOM	1913	CB	ASN A 470	-6.609	3.402	31.625	1.00	19.01		A	C
ANISOU	1913	CB	ASN A 470	2376	2508	2338	-26	117	73	A	C
ATOM	1916	CG	ASN A 470	-5.920	2.322	30.803	1.00	20.11		A	C
ANISOU	1916	CG	ASN A 470	2489	2427	2724	-4	42	-3	A	C
ATOM	1917	OD1	ASN A 470	-6.515	1.257	30.597	1.00	24.09		A	O
ANISOU	1917	OD1	ASN A 470	3081	2773	3298	-190	-36	-56	A	O
ATOM	1918	ND2	ASN A 470	-4.705	2.572	30.314	1.00	19.43		A	N
ANISOU	1918	ND2	ASN A 470	2535	2283	2564	-59	144	223	A	N
ATOM	1921	C	ASN A 470	-5.354	5.501	30.952	1.00	18.16		A	C
ANISOU	1921	C	ASN A 470	2259	2300	2339	13	120	181	A	C

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ATOM	1922	O	ASN A 470	-4.271	5.438	30.381	1.00	17.52		A	O
ANISOU	1922	O	ASN A 470	2168	2260	2226	80	174	145	A	O
ATOM	1923	N	ILE A 471	-6.265	6.424	30.653	1.00	17.12		A	N
ANISOU	1923	N	ILE A 471	2078	2184	2240	24	147	178	A	N
ATOM	1925	CA	ILE A 471	-5.987	7.398	29.584	1.00	16.44		A	C
ANISOU	1925	CA	ILE A 471	2045	2096	2103	35	23	127	A	C
ATOM	1927	CB	ILE A 471	-7.225	8.247	29.277	1.00	17.36		A	C
ANISOU	1927	CB	ILE A 471	2240	2155	2201	69	65	98	A	C
ATOM	1929	CG1	ILE A 471	-8.385	7.341	28.874	1.00	18.58		A	C
ANISOU	1929	CG1	ILE A 471	2291	2377	2390	28	-40	21	A	C
ATOM	1932	CD1	ILE A 471	-9.658	8.059	28.581	1.00	20.35		A	C
ANISOU	1932	CD1	ILE A 471	2448	2552	2730	-29	15	131	A	C
ATOM	1936	CG2	ILE A 471	-6.926	9.278	28.160	1.00	17.48		A	C
ANISOU	1936	CG2	ILE A 471	2100	2192	2347	16	117	89	A	C
ATOM	1940	C	ILE A 471	-4.839	8.308	30.046	1.00	16.39		A	C
ANISOU	1940	C	ILE A 471	2079	2010	2135	35	52	84	A	C
ATOM	1941	O	ILE A 471	-3.921	8.622	29.263	1.00	16.29		A	O
ANISOU	1941	O	ILE A 471	2030	2000	2157	-64	101	194	A	O
ATOM	1942	N	ILE A 472	-4.879	8.716	31.309	1.00	15.92		A	N
ANISOU	1942	N	ILE A 472	2016	2007	2024	5	91	187	A	N
ATOM	1944	CA	ILE A 472	-3.849	9.570	31.861	1.00	16.08		A	C
ANISOU	1944	CA	ILE A 472	2100	2037	1970	49	37	47	A	C
ATOM	1946	CB	ILE A 472	-4.225	10.069	33.286	1.00	16.07		A	C
ANISOU	1946	CB	ILE A 472	2158	2132	1814	17	-2	116	A	C
ATOM	1948	CG1	ILE A 472	-5.536	10.865	33.258	1.00	17.87		A	C
ANISOU	1948	CG1	ILE A 472	2295	2339	2153	0	124	17	A	C
ATOM	1951	CD1	ILE A 472	-6.206	10.979	34.642	1.00	19.82		A	C
ANISOU	1951	CD1	ILE A 472	2615	2582	2332	135	52	84	A	C
ATOM	1955	CG2	ILE A 472	-3.119	10.869	33.899	1.00	15.68		A	C
ANISOU	1955	CG2	ILE A 472	2095	2068	1793	63	100	284	A	C
ATOM	1959	C	ILE A 472	-2.497	8.855	31.857	1.00	15.21		A	C
ANISOU	1959	C	ILE A 472	1970	1924	1883	26	28	12	A	C
ATOM	1960	O	ILE A 472	-1.462	9.435	31.500	1.00	15.59		A	O
ANISOU	1960	O	ILE A 472	2141	1849	1930	25	-14	70	A	O
ATOM	1961	N	GLU A 473	-2.513	7.569	32.215	1.00	15.53		A	N
ANISOU	1961	N	GLU A 473	1971	1948	1981	50	62	137	A	N
ATOM	1963	CA	GLU A 473	-1.288	6.754	32.192	1.00	15.53		A	C
ANISOU	1963	CA	GLU A 473	2027	1971	1901	49	77	61	A	C
ATOM	1965	CB	GLU A 473	-1.636	5.317	32.558	1.00	16.54		A	C
ANISOU	1965	CB	GLU A 473	2214	2001	2066	38	-9	25	A	C
ATOM	1968	CG	GLU A 473	-0.498	4.324	32.531	1.00	17.12		A	C
ANISOU	1968	CG	GLU A 473	2111	2294	2100	23	-57	10	A	C
ATOM	1971	CD	GLU A 473	-0.984	2.900	32.768	1.00	20.65		A	C
ANISOU	1971	CD	GLU A 473	2713	2498	2632	-13	-65	40	A	C
ATOM	1972	OE1	GLU A 473	-2.154	2.586	32.414	1.00	20.93		A	O
ANISOU	1972	OE1	GLU A 473	2839	2411	2699	22	25	72	A	O
ATOM	1973	OE2	GLU A 473	-0.178	2.102	33.308	1.00	23.11		A	O
ANISOU	1973	OE2	GLU A 473	3091	2620	3068	152	125	199	A	O
ATOM	1974	C	GLU A 473	-0.636	6.792	30.785	1.00	14.88		A	C
ANISOU	1974	C	GLU A 473	1965	1817	1870	-7	79	36	A	C
ATOM	1975	O	GLU A 473	0.550	7.033	30.650	1.00	15.07		A	O
ANISOU	1975	O	GLU A 473	1986	1877	1859	77	38	68	A	O
ATOM	1976	N	LEU A 474	-1.453	6.587	29.769	1.00	14.31		A	N
ANISOU	1976	N	LEU A 474	1895	1751	1791	28	70	103	A	N
ATOM	1978	CA	LEU A 474	-0.971	6.514	28.393	1.00	14.03		A	C
ANISOU	1978	CA	LEU A 474	1903	1689	1739	-34	25	57	A	C
ATOM	1980	CB	LEU A 474	-2.077	5.971	27.482	1.00	13.65		A	C
ANISOU	1980	CB	LEU A 474	1770	1654	1760	-17	96	115	A	C
ATOM	1983	CG	LEU A 474	-2.519	4.537	27.818	1.00	15.57		A	C
ANISOU	1983	CG	LEU A 474	1988	1912	2013	-93	59	124	A	C
ATOM	1985	CD1	LEU A 474	-3.767	4.219	27.029	1.00	17.03		A	C
ANISOU	1985	CD1	LEU A 474	2124	2142	2204	-146	-4	39	A	C

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Figure 1A – 32

ATOM	1989	CD2	LEU	A	474	-1.396	3.526	27.529	1.00	17.65		A	C
ANISOU	1989	CD2	LEU	A	474	2332	2071	2300	41	19	65	A	C
ATOM	1993	C	LEU	A	474	-0.449	7.866	27.906	1.00	14.40		A	C
ANISOU	1993	C	LEU	A	474	1827	1836	1808	-38	3	76	A	C
ATOM	1994	O	LEU	A	474	0.622	7.943	27.283	1.00	14.36		A	O
ANISOU	1994	O	LEU	A	474	1829	1888	1739	-75	100	58	A	O
ATOM	1995	N	VAL	A	475	-1.208	8.927	28.158	1.00	14.39		A	N
ANISOU	1995	N	VAL	A	475	1822	1839	1806	-49	-17	-22	A	N
ATOM	1997	CA	VAL	A	475	-0.729	10.225	27.693	1.00	14.60		A	C
ANISOU	1997	CA	VAL	A	475	1854	1850	1842	-12	-26	64	A	C
ATOM	1999	CB	VAL	A	475	-1.812	11.334	27.622	1.00	16.08		A	C
ANISOU	1999	CB	VAL	A	475	1981	2061	2067	-18	-60	26	A	C
ATOM	2001	CG1	VAL	A	475	-2.853	10.953	26.579	1.00	16.80		A	C
ANISOU	2001	CG1	VAL	A	475	2143	2215	2023	-6	-89	-13	A	C
ATOM	2005	CG2	VAL	A	475	-2.407	11.620	28.924	1.00	17.24		A	C
ANISOU	2005	CG2	VAL	A	475	2025	2296	2229	66	-2	117	A	C
ATOM	2009	C	VAL	A	475	0.514	10.656	28.471	1.00	13.49		A	C
ANISOU	2009	C	VAL	A	475	1696	1718	1708	17	11	92	A	C
ATOM	2010	O	VAL	A	475	1.370	11.343	27.922	1.00	13.18		A	O
ANISOU	2010	O	VAL	A	475	1596	1552	1857	14	23	121	A	O
ATOM	2011	N	HIS	A	476	0.599	10.284	29.757	1.00	13.15		A	N
ANISOU	2011	N	HIS	A	476	1686	1706	1603	-80	-7	53	A	N
ATOM	2013	CA	HIS	A	476	1.800	10.537	30.517	1.00	13.14		A	C
ANISOU	2013	CA	HIS	A	476	1750	1679	1564	30	27	78	A	C
ATOM	2015	CB	HIS	A	476	1.614	10.188	31.998	1.00	13.28		A	C
ANISOU	2015	CB	HIS	A	476	1841	1636	1568	42	-24	50	A	C
ATOM	2018	CG	HIS	A	476	2.873	10.341	32.767	1.00	13.64		A	C
ANISOU	2018	CG	HIS	A	476	1888	1755	1538	41	-2	40	A	C
ATOM	2019	ND1	HIS	A	476	3.476	9.300	33.450	1.00	16.28		A	N
ANISOU	2019	ND1	HIS	A	476	2335	1938	1912	114	-67	139	A	N
ATOM	2021	CE1	HIS	A	476	4.610	9.738	33.973	1.00	15.70		A	C
ANISOU	2021	CE1	HIS	A	476	2204	1900	1861	97	-30	73	A	C
ATOM	2023	NE2	HIS	A	476	4.751	11.019	33.675	1.00	15.65		A	N
ANISOU	2023	NE2	HIS	A	476	2238	2020	1687	123	-57	208	A	N
ATOM	2025	CD2	HIS	A	476	3.688	11.407	32.901	1.00	14.41		A	C
ANISOU	2025	CD2	HIS	A	476	1961	1724	1790	-18	-112	1	A	C
ATOM	2027	C	HIS	A	476	3.010	9.815	29.894	1.00	13.20		A	C
ANISOU	2027	C	HIS	A	476	1777	1695	1544	12	31	30	A	C
ATOM	2028	O	HIS	A	476	4.102	10.385	29.802	1.00	13.90		A	O
ANISOU	2028	O	HIS	A	476	1814	1735	1729	127	-59	-60	A	O
ATOM	2029	N	GLN	A	477	2.821	8.571	29.456	1.00	12.35		A	N
ANISOU	2029	N	GLN	A	477	1601	1541	1550	1	9	61	A	N
ATOM	2031	CA	GLN	A	477	3.910	7.879	28.754	1.00	12.50		A	C
ANISOU	2031	CA	GLN	A	477	1651	1519	1577	42	-45	28	A	C
ATOM	2033	CB	GLN	A	477	3.521	6.436	28.399	1.00	12.99		A	C
ANISOU	2033	CB	GLN	A	477	1665	1585	1683	-36	-22	67	A	C
ATOM	2036	CG	GLN	A	477	3.412	5.573	29.644	1.00	14.08		A	C
ANISOU	2036	CG	GLN	A	477	1850	1769	1729	25	-42	120	A	C
ATOM	2039	CD	GLN	A	477	2.706	4.252	29.424	1.00	15.11		A	C
ANISOU	2039	CD	GLN	A	477	2147	1742	1851	-44	-22	108	A	C
ATOM	2040	OE1	GLN	A	477	2.104	4.016	28.376	1.00	17.06		A	O
ANISOU	2040	OE1	GLN	A	477	2594	1851	2036	-60	-19	189	A	O
ATOM	2041	NE2	GLN	A	477	2.749	3.378	30.467	1.00	17.26		A	N
ANISOU	2041	NE2	GLN	A	477	2622	1782	2153	-195	6	321	A	N
ATOM	2044	C	GLN	A	477	4.357	8.652	27.520	1.00	12.85		A	C
ANISOU	2044	C	GLN	A	477	1622	1612	1647	-36	-21	22	A	C
ATOM	2045	O	GLN	A	477	5.542	8.810	27.262	1.00	13.58		A	O
ANISOU	2045	O	GLN	A	477	1605	1822	1733	123	-146	115	A	O
ATOM	2046	N	VAL	A	478	3.400	9.134	26.738	1.00	13.11		A	N
ANISOU	2046	N	VAL	A	478	1699	1615	1667	11	-38	14	A	N
ATOM	2048	CA	VAL	A	478	3.731	9.966	25.588	1.00	12.51		A	C
ANISOU	2048	CA	VAL	A	478	1707	1559	1487	52	-25	-14	A	C



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ATOM	2050	CB	VAL	A	478	2.477	10.397	24.816	1.00	12.75		A	C
ANISOU	2050	CB	VAL	A	478	1716	1612	1516	63	21	48	A	C
ATOM	2052	CG1	VAL	A	478	2.827	11.354	23.665	1.00	13.01		A	C
ANISOU	2052	CG1	VAL	A	478	1793	1682	1467	-17	60	-25	A	C
ATOM	2056	CG2	VAL	A	478	1.730	9.214	24.279	1.00	12.84		A	C
ANISOU	2056	CG2	VAL	A	478	1750	1740	1388	95	-3	94	A	C
ATOM	2060	C	VAL	A	478	4.568	11.177	26.045	1.00	12.91		A	C
ANISOU	2060	C	VAL	A	478	1700	1662	1543	63	-91	33	A	C
ATOM	2061	O	VAL	A	478	5.551	11.526	25.402	1.00	13.77		A	O
ANISOU	2061	O	VAL	A	478	1846	1825	1561	96	-85	-18	A	O
ATOM	2062	N	SER	A	479	4.180	11.830	27.155	1.00	13.21		A	N
ANISOU	2062	N	SER	A	479	1773	1677	1567	46	-73	18	A	N
ATOM	2064	CA	SER	A	479	4.936	12.990	27.624	1.00	13.01		A	C
ANISOU	2064	CA	SER	A	479	1686	1641	1616	9	-50	85	A	C
ATOM	2066	CB	SER	A	479	4.219	13.745	28.760	1.00	13.08		A	C
ANISOU	2066	CB	SER	A	479	1692	1636	1638	-37	8	86	A	C
ATOM	2069	OG	SER	A	479	4.270	13.067	30.004	1.00	14.85		A	O
ANISOU	2069	OG	SER	A	479	1992	1881	1767	-34	-135	155	A	O
ATOM	2071	C	SER	A	479	6.346	12.605	28.049	1.00	13.43		A	C
ANISOU	2071	C	SER	A	479	1738	1702	1664	40	-43	27	A	C
ATOM	2072	O	SER	A	479	7.249	13.404	27.908	1.00	13.82		A	O
ANISOU	2072	O	SER	A	479	1695	1790	1764	38	-155	83	A	O
ATOM	2073	N	MET	A	480	6.532	11.388	28.560	1.00	13.58		A	N
ANISOU	2073	N	MET	A	480	1744	1670	1743	-62	10	71	A	N
ATOM	2075	CA	MET	A	480	7.890	10.937	28.894	1.00	14.28		A	C
ANISOU	2075	CA	MET	A	480	1862	1759	1805	40	-66	44	A	C
ATOM	2077	CB	MET	A	480	7.875	9.656	29.764	1.00	14.20		A	C
ANISOU	2077	CB	MET	A	480	1825	1725	1844	94	-72	79	A	C
ATOM	2080	CG	MET	A	480	7.392	9.904	31.173	1.00	15.51		A	C
ANISOU	2080	CG	MET	A	480	1911	1968	2014	-12	-34	115	A	C
ATOM	2083	SD	MET	A	480	7.499	8.525	32.276	1.00	19.02		A	S
ANISOU	2083	SD	MET	A	480	2642	2364	2220	270	-125	329	A	S
ATOM	2084	CE	MET	A	480	6.215	7.580	31.747	1.00	18.10		A	C
ANISOU	2084	CE	MET	A	480	2459	2306	2111	191	-20	252	A	C
ATOM	2088	C	MET	A	480	8.728	10.735	27.646	1.00	14.18		A	C
ANISOU	2088	C	MET	A	480	1788	1766	1834	66	-103	71	A	C
ATOM	2089	O	MET	A	480	9.893	11.133	27.586	1.00	14.84		A	O
ANISOU	2089	O	MET	A	480	1940	1876	1820	38	-143	146	A	O
ATOM	2090	N	GLY	A	481	8.126	10.127	26.622	1.00	13.43		A	N
ANISOU	2090	N	GLY	A	481	1776	1603	1723	97	-36	-10	A	N
ATOM	2092	CA	GLY	A	481	8.808	9.952	25.354	1.00	13.56		A	C
ANISOU	2092	CA	GLY	A	481	1678	1734	1739	67	-7	4	A	C
ATOM	2095	C	GLY	A	481	9.185	11.300	24.733	1.00	13.51		A	C
ANISOU	2095	C	GLY	A	481	1691	1800	1642	66	-2	42	A	C
ATOM	2096	O	GLY	A	481	10.275	11.490	24.181	1.00	14.09		A	O
ANISOU	2096	O	GLY	A	481	1712	1857	1783	146	45	82	A	O
ATOM	2097	N	MET	A	482	8.267	12.263	24.799	1.00	13.36		A	N
ANISOU	2097	N	MET	A	482	1650	1710	1713	70	-34	5	A	N
ATOM	2099	CA	MET	A	482	8.514	13.582	24.263	1.00	13.04		A	C
ANISOU	2099	CA	MET	A	482	1574	1729	1648	60	-3	48	A	C
ATOM	2101	CB	MET	A	482	7.211	14.367	24.109	1.00	12.60		A	C
ANISOU	2101	CB	MET	A	482	1445	1699	1642	20	48	53	A	C
ATOM	2104	CG	MET	A	482	6.315	13.806	23.021	1.00	13.04		A	C
ANISOU	2104	CG	MET	A	482	1623	1652	1678	-17	-1	45	A	C
ATOM	2107	SD	MET	A	482	7.041	13.599	21.398	1.00	14.61		A	S
ANISOU	2107	SD	MET	A	482	1763	1904	1885	22	-48	5	A	S
ATOM	2108	CE	MET	A	482	7.516	15.235	21.059	1.00	16.31		A	C
ANISOU	2108	CE	MET	A	482	2129	1939	2127	112	-49	64	A	C
ATOM	2112	C	MET	A	482	9.535	14.381	25.080	1.00	13.08		A	C
ANISOU	2112	C	MET	A	482	1544	1660	1765	81	-48	83	A	C
ATOM	2113	O	MET	A	482	10.303	15.147	24.511	1.00	13.77		A	O
ANISOU	2113	O	MET	A	482	1605	1802	1824	107	-42	195	A	O

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ATOM	2114	N	LYS	A	483	9.530	14.242	26.406	1.00	13.90		A	N
ANISOU	2114	N	LYS	A	483	1668	1807	1806	39	7	47	A	N
ATOM	2116	CA	LYS	A	483	10.563	14.844	27.240	1.00	15.25		A	C
ANISOU	2116	CA	LYS	A	483	1884	1902	2007	34	-62	82	A	C
ATOM	2118	CB	LYS	A	483	10.301	14.522	28.725	1.00	16.21		A	C
ANISOU	2118	CB	LYS	A	483	1994	2119	2043	57	-27	-17	A	C
ATOM	2121	CG	ALYS	A	483	11.324	15.117	29.688	0.50	18.03		A	C
ANISOU	2121	CG	ALYS	A	483	2171	2324	2354	5	-65	-50	A	C
ATOM	2122	CG	BLYS	A	483	11.270	15.200	29.692	0.50	17.57		A	C
ANISOU	2122	CG	BLYS	A	483	2129	2241	2304	17	-56	-40	A	C
ATOM	2127	CD	ALYS	A	483	11.077	14.657	31.111	0.50	21.05		A	C
ANISOU	2127	CD	ALYS	A	483	2664	2760	2572	-15	-5	14	A	C
ATOM	2128	CD	BLYS	A	483	10.968	14.846	31.136	0.50	20.23		A	C
ANISOU	2128	CD	BLYS	A	483	2545	2652	2488	6	-14	20	A	C
ATOM	2133	CE	ALYS	A	483	12.283	14.936	32.014	0.50	23.51		A	C
ANISOU	2133	CE	ALYS	A	483	2798	3184	2950	43	-62	29	A	C
ATOM	2134	CE	BLYS	A	483	12.056	15.382	32.082	0.50	21.97		A	C
ANISOU	2134	CE	BLYS	A	483	2793	2811	2744	-29	-15	6	A	C
ATOM	2139	NZ	ALYS	A	483	11.915	14.913	33.457	0.50	25.90		A	N
ANISOU	2139	NZ	ALYS	A	483	3254	3519	3064	47	-55	2	A	N
ATOM	2140	NZ	BLYS	A	483	13.356	14.734	31.770	0.50	24.42		A	N
ANISOU	2140	NZ	BLYS	A	483	2987	3170	3119	24	6	-85	A	N
ATOM	2147	C	LYS	A	483	11.949	14.358	26.761	1.00	14.71		A	C
ANISOU	2147	C	LYS	A	483	1892	1869	1827	10	-44	-6	A	C
ATOM	2148	O	LYS	A	483	12.893	15.128	26.654	1.00	15.16		A	O
ANISOU	2148	O	LYS	A	483	1785	1991	1982	110	-82	80	A	O
ATOM	2149	N	TYR	A	484	12.036	13.079	26.435	1.00	15.05		A	N
ANISOU	2149	N	TYR	A	484	1804	1916	1997	148	-32	83	A	N
ATOM	2151	CA	TYR	A	484	13.279	12.492	25.915	1.00	15.15		A	C
ANISOU	2151	CA	TYR	A	484	1820	1989	1945	55	30	51	A	C
ATOM	2153	CB	TYR	A	484	13.151	10.982	25.798	1.00	15.90		A	C
ANISOU	2153	CB	TYR	A	484	1908	2086	2047	126	-9	64	A	C
ATOM	2156	CG	TYR	A	484	14.275	10.360	25.006	1.00	15.20		A	C
ANISOU	2156	CG	TYR	A	484	1765	1981	2028	-21	126	78	A	C
ATOM	2157	CD1	TYR	A	484	15.537	10.218	25.567	1.00	18.84		A	C
ANISOU	2157	CD1	TYR	A	484	2332	2557	2266	122	-80	-30	A	C
ATOM	2159	CE1	TYR	A	484	16.551	9.665	24.844	1.00	19.20		A	C
ANISOU	2159	CE1	TYR	A	484	2021	2698	2574	190	-62	56	A	C
ATOM	2161	CZ	TYR	A	484	16.341	9.293	23.550	1.00	19.05		A	C
ANISOU	2161	CZ	TYR	A	484	2226	2444	2567	187	-11	-40	A	C
ATOM	2162	OH	TYR	A	484	17.343	8.728	22.791	1.00	22.46		A	O
ANISOU	2162	OH	TYR	A	484	2426	3071	3035	64	264	-205	A	O
ATOM	2164	CE2	TYR	A	484	15.109	9.435	22.974	1.00	18.31		A	C
ANISOU	2164	CE2	TYR	A	484	2139	2503	2315	46	145	-87	A	C
ATOM	2166	CD2	TYR	A	484	14.099	9.986	23.712	1.00	15.22		A	C
ANISOU	2166	CD2	TYR	A	484	1705	1923	2153	113	1	171	A	C
ATOM	2168	C	TYR	A	484	13.649	13.086	24.571	1.00	15.05		A	C
ANISOU	2168	C	TYR	A	484	1787	1956	1975	33	-11	52	A	C
ATOM	2169	O	TYR	A	484	14.787	13.446	24.359	1.00	16.24		A	O
ANISOU	2169	O	TYR	A	484	1733	2198	2238	80	-53	201	A	O
ATOM	2170	N	LEU	A	485	12.688	13.211	23.670	1.00	14.71		A	N
ANISOU	2170	N	LEU	A	485	1783	1858	1947	77	2	76	A	N
ATOM	2172	CA	LEU	A	485	12.972	13.756	22.369	1.00	14.83		A	C
ANISOU	2172	CA	LEU	A	485	1753	1964	1916	39	-34	27	A	C
ATOM	2174	CB	LEU	A	485	11.713	13.681	21.496	1.00	15.89		A	C
ANISOU	2174	CB	LEU	A	485	1880	2104	2052	58	-48	22	A	C
ATOM	2177	CG	ALEU	A	485	11.413	12.379	20.736	0.70	17.45		A	C
ANISOU	2177	CG	ALEU	A	485	2100	2287	2241	0	-12	-65	A	C
ATOM	2178	CG	BLEU	A	485	11.906	13.807	19.982	0.30	15.27		A	C
ANISOU	2178	CG	BLEU	A	485	1854	1933	2013	55	-5	53	A	C
ATOM	2181	CD1ALEU	A	485	10.116	12.377	19.970	0.70	17.55			A	C
ANISOU	2181	CD1ALEU	A	485	2133	2366	2165	36	-38	-103		A	C

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Figure 1A – 35

ATOM	2182	CD1BLEU	A	485	12.784	12.756	19.299	0.30	16.08		A	C	
ANISOU	2182	CD1BLEU	A	485	2037	2028	2044	67	35	50	A	C	
ATOM	2189	CD2ALEU	A	485	12.558	11.840	19.865	0.70	17.41		A	C	
ANISOU	2189	CD2ALEU	A	485	1992	2217	2404	46	44	-130	A	C	
ATOM	2190	CD2BLEU	A	485	10.586	14.084	19.224	0.30	15.19		A	C	
ANISOU	2190	CD2BLEU	A	485	1864	2020	1887	-76	-57	17	A	C	
ATOM	2197	C	LEU	A	485	13.420	15.199	22.498	1.00	15.63		A	C
ANISOU	2197	C	LEU	A	485	1860	2068	2008	27	-57	57	A	C
ATOM	2198	O	LEU	A	485	14.321	15.623	21.770	1.00	16.27		A	O
ANISOU	2198	O	LEU	A	485	1742	2287	2152	20	-46	116	A	O
ATOM	2199	N	GLU	A	486	12.781	15.950	23.405	1.00	14.60		A	N
ANISOU	2199	N	GLU	A	486	1708	1946	1892	20	-81	71	A	N
ATOM	2201	CA	GLU	A	486	13.141	17.354	23.615	1.00	15.01		A	C
ANISOU	2201	CA	GLU	A	486	1807	1973	1923	81	-75	35	A	C
ATOM	2203	CB	GLU	A	486	12.132	18.002	24.585	1.00	16.14		A	C
ANISOU	2203	CB	GLU	A	486	1881	2159	2091	5	-97	14	A	C
ATOM	2206	CG	GLU	A	486	12.462	19.394	25.047	1.00	16.65		A	C
ANISOU	2206	CG	GLU	A	486	1998	2103	2225	90	-52	86	A	C
ATOM	2209	CD	GLU	A	486	11.443	19.852	26.055	1.00	18.29		A	C
ANISOU	2209	CD	GLU	A	486	2328	2281	2337	20	-17	-96	A	C
ATOM	2210	OE1	GLU	A	486	11.564	19.554	27.264	1.00	20.63		A	O
ANISOU	2210	OE1	GLU	A	486	2302	2944	2590	39	-118	176	A	O
ATOM	2211	OE2	GLU	A	486	10.473	20.450	25.618	1.00	17.98		A	O
ANISOU	2211	OE2	GLU	A	486	1932	2456	2441	-97	-127	-10	A	O
ATOM	2212	C	GLU	A	486	14.582	17.431	24.152	1.00	15.93		A	C
ANISOU	2212	C	GLU	A	486	1890	2038	2124	-31	-36	36	A	C
ATOM	2213	O	GLU	A	486	15.373	18.240	23.696	1.00	15.99		A	O
ANISOU	2213	O	GLU	A	486	1501	2336	2238	27	-28	170	A	O
ATOM	2214	N	GLU	A	487	14.901	16.589	25.132	1.00	16.37		A	N
ANISOU	2214	N	GLU	A	487	1924	2153	2141	23	-41	132	A	N
ATOM	2216	CA	GLU	A	487	16.267	16.529	25.674	1.00	18.39		A	C
ANISOU	2216	CA	GLU	A	487	2166	2429	2393	-14	-42	42	A	C
ATOM	2218	CB	GLU	A	487	16.370	15.544	26.847	1.00	19.56		A	C
ANISOU	2218	CB	GLU	A	487	2334	2580	2518	-32	-64	64	A	C
ATOM	2221	CG	AGLU	A	487	17.595	14.659	26.907	0.40	21.52		A	C
ANISOU	2221	CG	AGLU	A	487	2586	2733	2857	42	-25	16	A	C
ATOM	2222	CG	BGLU	A	487	15.559	15.856	28.083	0.60	20.39		A	C
ANISOU	2222	CG	BGLU	A	487	2453	2686	2605	2	-8	65	A	C
ATOM	2227	CD	AGLU	A	487	17.696	13.956	28.248	0.40	24.13		A	C
ANISOU	2227	CD	AGLU	A	487	3000	3116	3052	-21	-17	116	A	C
ATOM	2228	CD	BGLU	A	487	15.400	14.633	28.998	0.60	21.01		A	C
ANISOU	2228	CD	BGLU	A	487	2635	2678	2668	16	-44	106	A	C
ATOM	2229	OE1AGLU	A	487	17.756	12.713	28.262	0.40	24.53		A	O	
ANISOU	2229	OE1AGLU	A	487	3039	3126	3154	-39	-58	71	A	O	
ATOM	2230	OE1BGLU	A	487	15.601	13.509	28.505	0.60	22.61		A	O	
ANISOU	2230	OE1BGLU	A	487	2839	2906	2846	-59	-67	85	A	O	
ATOM	2231	OE2AGLU	A	487	17.727	14.649	29.289	0.60	28.92		A	O	
ANISOU	2231	OE2AGLU	A	487	3757	3572	3657	10	28	-90	A	O	
ATOM	2232	OE2BGLU	A	487	15.075	14.801	30.203	0.40	20.19		A	O	
ANISOU	2232	OE2BGLU	A	487	2354	2605	2712	-40	-35	38	A	O	
ATOM	2233	C	GLU	A	487	17.335	16.202	24.609	1.00	18.09		A	C
ANISOU	2233	C	GLU	A	487	2155	2411	2307	-32	-52	66	A	C
ATOM	2234	O	GLU	A	487	18.477	16.655	24.699	1.00	18.91		A	O
ANISOU	2234	O	GLU	A	487	2116	2668	2400	-31	-28	176	A	O
ATOM	2235	N	SER	A	488	16.935	15.400	23.636	1.00	17.43		A	N
ANISOU	2235	N	SER	A	488	2088	2302	2233	73	-37	48	A	N
ATOM	2237	CA	SER	A	488	17.752	14.916	22.558	1.00	17.60		A	C
ANISOU	2237	CA	SER	A	488	2125	2328	2232	35	-47	74	A	C
ATOM	2239	CB	SER	A	488	17.173	13.592	22.091	1.00	18.02		A	C
ANISOU	2239	CB	SER	A	488	2169	2407	2268	31	-126	72	A	C
ATOM	2242	OG	SER	A	488	17.176	12.614	23.134	1.00	19.41		A	O
ANISOU	2242	OG	SER	A	488	2257	2387	2730	79	36	178	A	O

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ATOM	2244	C	SER	A	488	17.769	15.883	21.381	1.00	17.25		A	C
ANISOU	2244	C	SER	A	488	2119	2217	2216	35	-27	50	A	C
ATOM	2245	O	SER	A	488	18.428	15.629	20.380	1.00	18.35		A	O
ANISOU	2245	O	SER	A	488	2091	2524	2355	89	-42	77	A	O
ATOM	2246	N	ASN	A	489	16.980	16.944	21.473	1.00	17.54		A	N
ANISOU	2246	N	ASN	A	489	2075	2326	2260	110	1	88	A	N
ATOM	2248	CA	ASN	A	489	16.884	17.973	20.440	1.00	17.74		A	C
ANISOU	2248	CA	ASN	A	489	2151	2307	2281	17	0	34	A	C
ATOM	2250	CB	ASN	A	489	18.132	18.828	20.407	1.00	18.60		A	C
ANISOU	2250	CB	ASN	A	489	2236	2364	2464	50	-69	32	A	C
ATOM	2253	CG	ASN	A	489	18.139	19.832	21.553	1.00	21.17		A	C
ANISOU	2253	CG	ASN	A	489	2709	2554	2780	-7	-33	-47	A	C
ATOM	2254	OD1	ASN	A	489	17.107	20.492	21.833	1.00	26.79		A	O
ANISOU	2254	OD1	ASN	A	489	3084	3498	3594	110	1	-253	A	O
ATOM	2255	ND2	ASN	A	489	19.245	19.933	22.239	1.00	24.42		A	N
ANISOU	2255	ND2	ASN	A	489	3020	3176	3081	-40	-210	72	A	N
ATOM	2258	C	ASN	A	489	16.418	17.507	19.079	1.00	16.69		A	C
ANISOU	2258	C	ASN	A	489	1974	2155	2211	65	-4	56	A	C
ATOM	2259	O	ASN	A	489	16.949	17.878	18.035	1.00	16.20		A	O
ANISOU	2259	O	ASN	A	489	1821	2221	2111	9	-155	32	A	O
ATOM	2260	N	PHE	A	490	15.400	16.657	19.115	1.00	15.77		A	N
ANISOU	2260	N	PHE	A	490	1912	2009	2067	23	4	11	A	N
ATOM	2262	CA	PHE	A	490	14.702	16.276	17.914	1.00	16.12		A	C
ANISOU	2262	CA	PHE	A	490	1858	2176	2091	47	38	16	A	C
ATOM	2264	CB	PHE	A	490	14.620	14.775	17.761	1.00	16.13		A	C
ANISOU	2264	CB	PHE	A	490	1838	2153	2137	39	1	10	A	C
ATOM	2267	CG	PHE	A	490	15.912	14.124	17.368	1.00	18.30		A	C
ANISOU	2267	CG	PHE	A	490	2157	2350	2443	9	76	-78	A	C
ATOM	2268	CD1	PHE	A	490	16.813	13.785	18.328	1.00	21.13		A	C
ANISOU	2268	CD1	PHE	A	490	2436	2731	2861	78	-19	7	A	C
ATOM	2270	CE1	PHE	A	490	18.015	13.191	17.984	1.00	20.58		A	C
ANISOU	2270	CE1	PHE	A	490	2445	2662	2711	111	-21	-121	A	C
ATOM	2272	CZ	PHE	A	490	18.300	12.969	16.696	1.00	18.38		A	C
ANISOU	2272	CZ	PHE	A	490	2124	2345	2511	40	160	57	A	C
ATOM	2274	CE2	PHE	A	490	17.423	13.294	15.710	1.00	19.29		A	C
ANISOU	2274	CE2	PHE	A	490	2278	2456	2595	82	105	0	A	C
ATOM	2276	CD2	PHE	A	490	16.214	13.887	16.048	1.00	20.04		A	C
ANISOU	2276	CD2	PHE	A	490	2265	2688	2660	54	72	-47	A	C
ATOM	2278	C	PHE	A	490	13.274	16.815	18.018	1.00	15.51		A	C
ANISOU	2278	C	PHE	A	490	1815	2055	2022	80	21	20	A	C
ATOM	2279	O	PHE	A	490	12.717	16.861	19.107	1.00	16.92		A	O
ANISOU	2279	O	PHE	A	490	1771	2447	2211	159	54	98	A	O
ATOM	2280	N	VAL	A	491	12.750	17.259	16.883	1.00	14.60		A	N
ANISOU	2280	N	VAL	A	491	1637	1883	2025	52	38	-3	A	N
ATOM	2282	CA	VAL	A	491	11.349	17.633	16.781	1.00	14.34		A	C
ANISOU	2282	CA	VAL	A	491	1628	1880	1938	28	23	0	A	C
ATOM	2284	CB	VAL	A	491	11.160	19.022	16.162	1.00	14.31		A	C
ANISOU	2284	CB	VAL	A	491	1628	1898	1909	7	19	48	A	C
ATOM	2286	CG1	VAL	A	491	11.705	20.069	17.095	1.00	15.89		A	C
ANISOU	2286	CG1	VAL	A	491	1894	1979	2163	-8	28	68	A	C
ATOM	2290	CG2	VAL	A	491	11.804	19.157	14.838	1.00	15.17		A	C
ANISOU	2290	CG2	VAL	A	491	1759	1981	2023	-2	-23	7	A	C
ATOM	2294	C	VAL	A	491	10.600	16.562	16.001	1.00	14.25		A	C
ANISOU	2294	C	VAL	A	491	1696	1848	1870	2	76	-9	A	C
ATOM	2295	O	VAL	A	491	11.081	16.062	14.997	1.00	14.87		A	O
ANISOU	2295	O	VAL	A	491	1558	2133	1956	-93	83	-96	A	O
ATOM	2296	N	HIS	A	492	9.410	16.188	16.490	1.00	13.97		A	N
ANISOU	2296	N	HIS	A	492	1572	1882	1851	-18	39	-20	A	N
ATOM	2298	CA	HIS	A	492	8.623	15.142	15.866	1.00	13.62		A	C
ANISOU	2298	CA	HIS	A	492	1654	1734	1786	80	69	1	A	C
ATOM	2300	CB	HIS	A	492	7.662	14.542	16.880	1.00	13.02		A	C
ANISOU	2300	CB	HIS	A	492	1503	1789	1653	10	-51	152	A	C

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ATOM	2303	CG	HIS	A	492	6.989	13.311	16.405	1.00	13.84		A	C
ANISOU	2303	CG	HIS	A	492	1743	1803	1712	65	38	23	A	C
ATOM	2304	ND1	HIS	A	492	5.935	13.354	15.521	1.00	14.31		A	N
ANISOU	2304	ND1	HIS	A	492	1711	1934	1792	-54	-65	-4	A	N
ATOM	2306	CE1	HIS	A	492	5.551	12.115	15.252	1.00	15.94		A	C
ANISOU	2306	CE1	HIS	A	492	1994	1921	2140	-50	-99	74	A	C
ATOM	2308	NE2	HIS	A	492	6.322	11.271	15.925	1.00	13.34		A	N
ANISOU	2308	NE2	HIS	A	492	1602	1851	1616	-16	-34	-20	A	N
ATOM	2310	CD2	HIS	A	492	7.220	11.999	16.664	1.00	13.94		A	C
ANISOU	2310	CD2	HIS	A	492	1652	1827	1818	8	-163	7	A	C
ATOM	2312	C	HIS	A	492	7.846	15.622	14.677	1.00	13.57		A	C
ANISOU	2312	C	HIS	A	492	1644	1742	1768	-13	28	14	A	C
ATOM	2313	O	HIS	A	492	7.852	14.995	13.633	1.00	15.28		A	O
ANISOU	2313	O	HIS	A	492	1834	2055	1916	43	41	-18	A	O
ATOM	2314	N	ARG	A	493	7.102	16.701	14.874	1.00	13.66		A	N
ANISOU	2314	N	ARG	A	493	1627	1818	1743	112	26	-49	A	N
ATOM	2316	CA	ARG	A	493	6.344	17.348	13.802	1.00	14.33		A	C
ANISOU	2316	CA	ARG	A	493	1835	1853	1756	80	-4	-13	A	C
ATOM	2318	CB	ARG	A	493	7.266	17.733	12.650	1.00	14.69		A	C
ANISOU	2318	CB	ARG	A	493	1791	1890	1900	114	-2	83	A	C
ATOM	2321	CG	ARG	A	493	8.272	18.743	13.007	1.00	15.77		A	C
ANISOU	2321	CG	ARG	A	493	1954	2045	1993	48	-21	108	A	C
ATOM	2324	CD	ARG	A	493	9.131	19.178	11.866	1.00	17.24		A	C
ANISOU	2324	CD	ARG	A	493	2247	2216	2087	6	32	64	A	C
ATOM	2327	NE	ARG	A	493	8.430	19.956	10.851	1.00	16.98		A	N
ANISOU	2327	NE	ARG	A	493	2109	2091	2249	-62	-22	57	A	N
ATOM	2329	CZ	ARG	A	493	8.414	19.683	9.544	1.00	19.41		A	C
ANISOU	2329	CZ	ARG	A	493	2422	2547	2405	7	-9	-18	A	C
ATOM	2330	NH1	ARG	A	493	8.989	18.620	9.035	1.00	18.41		A	N
ANISOU	2330	NH1	ARG	A	493	2388	2291	2317	48	-94	280	A	N
ATOM	2333	NH2	ARG	A	493	7.803	20.512	8.723	1.00	21.50		A	N
ANISOU	2333	NH2	ARG	A	493	2833	2773	2564	191	71	92	A	N
ATOM	2336	C	ARG	A	493	5.145	16.601	13.260	1.00	13.79		A	C
ANISOU	2336	C	ARG	A	493	1621	1875	1744	89	66	6	A	C
ATOM	2337	O	ARG	A	493	4.534	17.048	12.277	1.00	15.01		A	O
ANISOU	2337	O	ARG	A	493	1771	2024	1905	75	-30	33	A	O
ATOM	2338	N	ASP	A	494	4.777	15.484	13.874	1.00	14.09		A	N
ANISOU	2338	N	ASP	A	494	1664	1877	1811	99	-47	-16	A	N
ATOM	2340	CA	ASP	A	494	3.537	14.797	13.511	1.00	13.40		A	C
ANISOU	2340	CA	ASP	A	494	1589	1795	1704	89	-42	-72	A	C
ATOM	2342	CB	ASP	A	494	3.778	13.853	12.325	1.00	14.55		A	C
ANISOU	2342	CB	ASP	A	494	1961	1828	1740	60	-78	-1	A	C
ATOM	2345	CG	ASP	A	494	2.512	13.530	11.577	1.00	16.60		A	C
ANISOU	2345	CG	ASP	A	494	2017	2248	2042	90	-31	-33	A	C
ATOM	2346	OD1	ASP	A	494	1.408	14.075	11.924	1.00	19.57		A	O
ANISOU	2346	OD1	ASP	A	494	2109	2726	2600	234	-258	151	A	O
ATOM	2347	OD2	ASP	A	494	2.537	12.692	10.649	1.00	20.43		A	O
ANISOU	2347	OD2	ASP	A	494	2694	2586	2483	52	-151	-203	A	O
ATOM	2348	C	ASP	A	494	2.931	14.088	14.731	1.00	13.81		A	C
ANISOU	2348	C	ASP	A	494	1590	1802	1855	89	-88	-33	A	C
ATOM	2349	O	ASP	A	494	2.432	12.952	14.681	1.00	15.01		A	O
ANISOU	2349	O	ASP	A	494	1699	2066	1935	89	-58	-64	A	O
ATOM	2350	N	LEU	A	495	2.953	14.796	15.850	1.00	13.39		A	N
ANISOU	2350	N	LEU	A	495	1557	1761	1769	86	-22	-16	A	N
ATOM	2352	CA	LEU	A	495	2.502	14.208	17.104	1.00	13.66		A	C
ANISOU	2352	CA	LEU	A	495	1526	1798	1865	24	38	-26	A	C
ATOM	2354	CB	LEU	A	495	3.166	14.897	18.292	1.00	13.21		A	C
ANISOU	2354	CB	LEU	A	495	1563	1725	1729	138	48	-14	A	C
ATOM	2357	CG	LEU	A	495	2.821	14.341	19.675	1.00	14.09		A	C
ANISOU	2357	CG	LEU	A	495	1646	1834	1871	59	122	71	A	C
ATOM	2359	CD1	LEU	A	495	3.218	12.859	19.774	1.00	15.28		A	C
ANISOU	2359	CD1	LEU	A	495	1916	2030	1857	99	90	60	A	C

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ATOM	2363	CD2	LEU	A	495	3.502	15.170	20.769	1.00	15.29		A	C
ANISOU	2363	CD2	LEU	A	495	1832	1930	2046	110	119	-70	A	C
ATOM	2367	C	LEU	A	495	0.996	14.319	17.145	1.00	13.95		A	C
ANISOU	2367	C	LEU	A	495	1551	1744	2003	101	-47	-12	A	C
ATOM	2368	O	LEU	A	495	0.460	15.403	17.101	1.00	18.46		A	O
ANISOU	2368	O	LEU	A	495	1985	1993	3032	50	-58	-163	A	O
ATOM	2369	N	ALA	A	496	0.338	13.182	17.133	1.00	13.37		A	N
ANISOU	2369	N	ALA	A	496	1482	1690	1906	82	47	6	A	N
ATOM	2371	CA	ALA	A	496	-1.121	13.098	17.105	1.00	13.21		A	C
ANISOU	2371	CA	ALA	A	496	1508	1706	1805	51	-43	11	A	C
ATOM	2373	CB	ALA	A	496	-1.596	13.221	15.686	1.00	13.63		A	C
ANISOU	2373	CB	ALA	A	496	1647	1759	1772	-8	94	-5	A	C
ATOM	2377	C	ALA	A	496	-1.514	11.738	17.624	1.00	13.47		A	C
ANISOU	2377	C	ALA	A	496	1547	1732	1838	51	-11	39	A	C
ATOM	2378	O	ALA	A	496	-0.707	10.791	17.588	1.00	14.05		A	O
ANISOU	2378	O	ALA	A	496	1569	1651	2116	103	-148	9	A	O
ATOM	2379	N	ALA	A	497	-2.753	11.576	18.048	1.00	14.34		A	N
ANISOU	2379	N	ALA	A	497	1656	1834	1957	27	-39	129	A	N
ATOM	2381	CA	ALA	A	497	-3.131	10.309	18.649	1.00	14.64		A	C
ANISOU	2381	CA	ALA	A	497	1786	1863	1910	12	-40	74	A	C
ATOM	2383	CB	ALA	A	497	-4.484	10.394	19.260	1.00	15.30		A	C
ANISOU	2383	CB	ALA	A	497	1903	1956	1950	-8	0	6	A	C
ATOM	2387	C	ALA	A	497	-3.045	9.157	17.642	1.00	15.17		A	C
ANISOU	2387	C	ALA	A	497	1879	1898	1986	-27	7	38	A	C
ATOM	2388	O	ALA	A	497	-2.792	8.018	18.020	1.00	15.30		A	O
ANISOU	2388	O	ALA	A	497	2006	1835	1969	-20	-81	90	A	O
ATOM	2389	N	ARG	A	498	-3.220	9.440	16.357	1.00	14.72		A	N
ANISOU	2389	N	ARG	A	498	1899	1794	1899	-23	-54	16	A	N
ATOM	2391	CA	ARG	A	498	-3.116	8.392	15.338	1.00	15.85		A	C
ANISOU	2391	CA	ARG	A	498	2016	1957	2047	7	-24	-30	A	C
ATOM	2393	CB	ARG	A	498	-3.558	8.933	13.963	1.00	17.21		A	C
ANISOU	2393	CB	ARG	A	498	2240	2176	2121	35	-89	-61	A	C
ATOM	2396	CG	ARG	A	498	-2.600	9.918	13.351	1.00	18.20		A	C
ANISOU	2396	CG	ARG	A	498	2312	2363	2239	17	-59	11	A	C
ATOM	2399	CD	ARG	A	498	-3.070	10.601	12.046	1.00	22.13		A	C
ANISOU	2399	CD	ARG	A	498	3046	2752	2610	35	-191	1	A	C
ATOM	2402	NE	ARG	A	498	-2.159	11.684	11.693	1.00	26.71		A	N
ANISOU	2402	NE	ARG	A	498	3466	3421	3258	36	0	189	A	N
ATOM	2404	CZ	ARG	A	498	-2.324	12.925	12.116	1.00	29.97		A	C
ANISOU	2404	CZ	ARG	A	498	3944	3724	3716	9	-16	4	A	C
ATOM	2405	NH1	ARG	A	498	-3.391	13.227	12.836	1.00	30.55		A	N
ANISOU	2405	NH1	ARG	A	498	3957	3829	3821	86	7	113	A	N
ATOM	2408	NH2	ARG	A	498	-1.466	13.880	11.787	1.00	32.69		A	N
ANISOU	2408	NH2	ARG	A	498	4103	4094	4223	-94	-84	50	A	N
ATOM	2411	C	ARG	A	498	-1.712	7.799	15.215	1.00	15.78		A	C
ANISOU	2411	C	ARG	A	498	2025	1968	2000	0	-10	-24	A	C
ATOM	2412	O	ARG	A	498	-1.544	6.707	14.652	1.00	17.00		A	O
ANISOU	2412	O	ARG	A	498	2169	2056	2233	-58	-40	-80	A	O
ATOM	2413	N	ASN	A	499	-0.717	8.536	15.703	1.00	15.30		A	N
ANISOU	2413	N	ASN	A	499	1949	1891	1970	27	-42	28	A	N
ATOM	2415	CA	ASN	A	499	0.685	8.147	15.653	1.00	15.14		A	C
ANISOU	2415	CA	ASN	A	499	1927	1933	1890	18	-18	15	A	C
ATOM	2417	CB	ASN	A	499	1.511	9.293	15.092	1.00	14.92		A	C
ANISOU	2417	CB	ASN	A	499	1799	1959	1910	60	-35	51	A	C
ATOM	2420	CG	ASN	A	499	1.262	9.508	13.628	1.00	16.54		A	C
ANISOU	2420	CG	ASN	A	499	2103	2057	2124	1	-85	37	A	C
ATOM	2421	OD1	ASN	A	499	0.821	8.580	12.931	1.00	17.78		A	O
ANISOU	2421	OD1	ASN	A	499	2556	1981	2217	-97	-52	-69	A	O
ATOM	2422	ND2	ASN	A	499	1.525	10.731	13.132	1.00	16.69		A	N
ANISOU	2422	ND2	ASN	A	499	2233	1815	2293	-136	-114	56	A	N
ATOM	2425	C	ASN	A	499	1.259	7.634	16.965	1.00	14.63		A	C
ANISOU	2425	C	ASN	A	499	1854	1804	1898	30	-14	-5	A	C

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## Figure 1A – 39

ATOM	2426	O	ASN A 499	2.451	7.386	17.065	1.00	15.91	A	O
ANISOU	2426	O	ASN A 499	1896	2303	1843	-2	-88	74	A O
ATOM	2427	N	VAL A 500	0.407	7.485	17.970	1.00	14.02	A	N
ANISOU	2427	N	VAL A 500	1766	1782	1776	-25	-50	52	A N
ATOM	2429	CA	VAL A 500	0.782	6.850	19.231	1.00	14.35	A	C
ANISOU	2429	CA	VAL A 500	1864	1729	1858	-10	-35	8	A C
ATOM	2431	CB	VAL A 500	0.203	7.597	20.425	1.00	14.12	A	C
ANISOU	2431	CB	VAL A 500	1865	1745	1753	20	-107	27	A C
ATOM	2433	CG1	VAL A 500	0.449	6.844	21.729	1.00	15.17	A	C
ANISOU	2433	CG1	VAL A 500	2182	1702	1878	-35	74	13	A C
ATOM	2437	CG2	VAL A 500	0.821	8.958	20.510	1.00	15.70	A	C
ANISOU	2437	CG2	VAL A 500	2260	1966	1738	-62	-175	32	A C
ATOM	2441	C	VAL A 500	0.204	5.432	19.141	1.00	15.00	A	C
ANISOU	2441	C	VAL A 500	1851	1842	2006	-52	-15	16	A C
ATOM	2442	O	VAL A 500	-0.994	5.270	18.933	1.00	15.41	A	O
ANISOU	2442	O	VAL A 500	1817	1871	2167	-5	-172	-78	A O
ATOM	2443	N	LEU A 501	1.055	4.436	19.371	1.00	15.14	A	N
ANISOU	2443	N	LEU A 501	1955	1831	1964	-16	-116	-62	A N
ATOM	2445	CA	LEU A 501	0.665	3.050	19.209	1.00	15.94	A	C
ANISOU	2445	CA	LEU A 501	2066	1918	2073	5	0	18	A C
ATOM	2447	CB	LEU A 501	1.545	2.394	18.186	1.00	15.51	A	C
ANISOU	2447	CB	LEU A 501	2015	1849	2029	41	-38	4	A C
ATOM	2450	CG	LEU A 501	1.615	3.035	16.813	1.00	17.11	A	C
ANISOU	2450	CG	LEU A 501	2221	2147	2132	86	94	19	A C
ATOM	2452	CD1	LEU A 501	2.717	2.364	15.968	1.00	17.91	A	C
ANISOU	2452	CD1	LEU A 501	2379	2248	2177	96	15	-153	A C
ATOM	2456	CD2	LEU A 501	0.265	2.915	16.153	1.00	19.70	A	C
ANISOU	2456	CD2	LEU A 501	2555	2566	2362	31	-54	-92	A C
ATOM	2460	C	LEU A 501	0.738	2.311	20.542	1.00	16.14	A	C
ANISOU	2460	C	LEU A 501	2087	1951	2092	56	-20	20	A C
ATOM	2461	O	LEU A 501	1.644	2.557	21.329	1.00	16.73	A	O
ANISOU	2461	O	LEU A 501	2254	1854	2248	42	-116	-33	A O
ATOM	2462	N	LEU A 502	-0.215	1.409	20.792	1.00	16.44	A	N
ANISOU	2462	N	LEU A 502	2209	1940	2097	-60	-34	-83	A N
ATOM	2464	CA	LEU A 502	-0.268	0.700	22.062	1.00	16.78	A	C
ANISOU	2464	CA	LEU A 502	2167	1998	2207	8	-3	1	A C
ATOM	2466	CB	LEU A 502	-1.718	0.531	22.512	1.00	17.49	A	C
ANISOU	2466	CB	LEU A 502	2293	2110	2242	30	22	86	A C
ATOM	2469	CG	LEU A 502	-2.396	1.827	22.962	1.00	22.15	A	C
ANISOU	2469	CG	LEU A 502	2723	2690	3000	133	133	-80	A C
ATOM	2471	CD1	LEU A 502	-3.726	1.503	23.597	1.00	23.84	A	C
ANISOU	2471	CD1	LEU A 502	2923	2936	3196	47	187	-38	A C
ATOM	2475	CD2	LEU A 502	-1.550	2.581	23.902	1.00	26.16	A	C
ANISOU	2475	CD2	LEU A 502	3225	3359	3353	25	-24	-117	A C
ATOM	2479	C	LEU A 502	0.400	-0.682	21.961	1.00	16.18	A	C
ANISOU	2479	C	LEU A 502	2112	1933	2099	12	18	-31	A C
ATOM	2480	O	LEU A 502	0.059	-1.465	21.090	1.00	16.94	A	O
ANISOU	2480	O	LEU A 502	2306	1898	2231	55	54	0	A O
ATOM	2481	N	VAL A 503	1.367	-0.935	22.836	1.00	16.34	A	N
ANISOU	2481	N	VAL A 503	2119	1892	2197	40	-4	-52	A N
ATOM	2483	CA	VAL A 503	1.992	-2.250	22.969	1.00	16.11	A	C
ANISOU	2483	CA	VAL A 503	2111	1883	2126	29	-4	-49	A C
ATOM	2485	CB	VAL A 503	3.360	-2.133	23.614	1.00	16.82	A	C
ANISOU	2485	CB	VAL A 503	2200	1909	2280	53	-66	7	A C
ATOM	2487	CG1	VAL A 503	3.982	-3.498	23.829	1.00	17.55	A	C
ANISOU	2487	CG1	VAL A 503	2118	2067	2481	103	-112	-21	A C
ATOM	2491	CG2	VAL A 503	4.277	-1.310	22.736	1.00	17.75	A	C
ANISOU	2491	CG2	VAL A 503	2173	2248	2321	165	19	-11	A C
ATOM	2495	C	VAL A 503	1.041	-3.105	23.810	1.00	17.67	A	C
ANISOU	2495	C	VAL A 503	2339	2044	2330	-23	-1	-33	A C
ATOM	2496	O	VAL A 503	0.819	-4.295	23.544	1.00	18.04	A	O
ANISOU	2496	O	VAL A 503	2513	1893	2448	-43	-29	-131	A O

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ATOM	2497	N	THR	A	504	0.535	-2.505	24.868	1.00	18.04		A	N
ANISOU	2497	N	THR	A	504	2356	2114	2382	-5	99	-3	A	N
ATOM	2499	CA	THR	A	504	-0.509	-3.091	25.699	1.00	18.50		A	C
ANISOU	2499	CA	THR	A	504	2374	2251	2405	-55	38	-1	A	C
ATOM	2501	CB	THR	A	504	0.025	-3.708	26.989	1.00	18.82		A	C
ANISOU	2501	CB	THR	A	504	2393	2309	2446	-26	6	24	A	C
ATOM	2503	OG1	THR	A	504	0.328	-2.667	27.946	1.00	19.92		A	O
ANISOU	2503	OG1	THR	A	504	2793	2293	2481	14	-28	56	A	O
ATOM	2505	CG2	THR	A	504	1.307	-4.492	26.742	1.00	19.30		A	C
ANISOU	2505	CG2	THR	A	504	2461	2310	2561	-24	55	7	A	C
ATOM	2509	C	THR	A	504	-1.463	-1.979	26.076	1.00	18.88		A	C
ANISOU	2509	C	THR	A	504	2407	2303	2460	-40	67	-19	A	C
ATOM	2510	O	THR	A	504	-1.275	-0.804	25.735	1.00	18.24		A	O
ANISOU	2510	O	THR	A	504	2291	2168	2468	-11	86	21	A	O
ATOM	2511	N	GLN	A	505	-2.506	-2.374	26.785	1.00	19.35		A	N
ANISOU	2511	N	GLN	A	505	2458	2324	2569	-101	102	-4	A	N
ATOM	2513	CA	GLN	A	505	-3.519	-1.464	27.241	1.00	20.34		A	C
ANISOU	2513	CA	GLN	A	505	2553	2533	2642	-47	56	8	A	C
ATOM	2515	CB	GLN	A	505	-4.665	-2.289	27.883	1.00	21.85		A	C
ANISOU	2515	CB	GLN	A	505	2668	2772	2859	-71	73	43	A	C
ATOM	2518	CG	AGLN	A	505	-5.220	-3.455	26.963	0.50	22.56		A	C
ANISOU	2518	CG	AGLN	A	505	2836	2832	2901	-36	4	2	A	C
ATOM	2519	CG	BGLN	A	505	-5.359	-1.513	28.981	0.50	23.42		A	C
ANISOU	2519	CG	BGLN	A	505	3047	2907	2942	-24	40	-15	A	C
ATOM	2524	CD	AGLN	A	505	-4.473	-4.821	26.820	0.50	23.64		A	C
ANISOU	2524	CD	AGLN	A	505	2917	2979	3086	18	-15	0	A	C
ATOM	2525	CD	BGLN	A	505	-6.797	-1.982	29.158	0.50	26.10		A	C
ANISOU	2525	CD	BGLN	A	505	3170	3288	3458	-14	29	-37	A	C
ATOM	2526	OE1	AGLN	A	505	-3.337	-5.008	27.232	0.50	19.90		A	O
ANISOU	2526	OE1	AGLN	A	505	2458	2174	2927	-264	141	108	A	O
ATOM	2527	OE1	BGLN	A	505	-7.052	-3.189	29.309	0.50	27.60		A	O
ANISOU	2527	OE1	BGLN	A	505	3362	3383	3740	-58	62	101	A	O
ATOM	2528	NE2	AGLN	A	505	-5.179	-5.787	26.208	0.50	26.91		A	N
ANISOU	2528	NE2	AGLN	A	505	3349	3392	3483	-106	-60	-51	A	N
ATOM	2529	NE2	BGLN	A	505	-7.743	-1.041	29.114	0.50	26.76		A	N
ANISOU	2529	NE2	BGLN	A	505	3217	3345	3603	14	-31	53	A	N
ATOM	2534	C	GLN	A	505	-2.903	-0.421	28.197	1.00	18.70		A	C
ANISOU	2534	C	GLN	A	505	2357	2287	2461	-42	110	57	A	C
ATOM	2535	O	GLN	A	505	-3.487	0.656	28.449	1.00	19.57		A	O
ANISOU	2535	O	GLN	A	505	2474	2432	2528	-28	204	-54	A	O
ATOM	2536	N	HIS	A	506	-1.712	-0.723	28.697	1.00	18.30		A	N
ANISOU	2536	N	HIS	A	506	2372	2176	2404	-91	89	42	A	N
ATOM	2538	CA	HIS	A	506	-1.014	0.135	29.648	1.00	17.71		A	C
ANISOU	2538	CA	HIS	A	506	2287	2226	2213	3	61	33	A	C
ATOM	2540	CB	HIS	A	506	-0.893	-0.586	30.993	1.00	18.19		A	C
ANISOU	2540	CB	HIS	A	506	2277	2287	2344	85	99	93	A	C
ATOM	2543	CG	HIS	A	506	-2.226	-0.864	31.597	1.00	20.26		A	C
ANISOU	2543	CG	HIS	A	506	2503	2537	2656	-42	163	157	A	C
ATOM	2544	ND1	HIS	A	506	-3.021	0.136	32.103	1.00	21.61		A	N
ANISOU	2544	ND1	HIS	A	506	2852	2585	2772	-15	169	118	A	N
ATOM	2546	CE1	HIS	A	506	-4.165	-0.384	32.509	1.00	24.41		A	C
ANISOU	2546	CE1	HIS	A	506	2980	3045	3246	1	171	73	A	C
ATOM	2548	NE2	HIS	A	506	-4.136	-1.684	32.288	1.00	23.91		A	N
ANISOU	2548	NE2	HIS	A	506	2812	2935	3336	-170	244	115	A	N
ATOM	2550	CD2	HIS	A	506	-2.927	-2.015	31.733	1.00	22.71		A	C
ANISOU	2550	CD2	HIS	A	506	2883	2672	3074	-74	177	46	A	C
ATOM	2552	C	HIS	A	506	0.376	0.573	29.180	1.00	16.96		A	C
ANISOU	2552	C	HIS	A	506	2239	2105	2099	-47	72	80	A	C
ATOM	2553	O	HIS	A	506	1.200	0.935	30.004	1.00	17.15		A	O
ANISOU	2553	O	HIS	A	506	2434	2094	1986	-169	228	70	A	O
ATOM	2554	N	TYR	A	507	0.637	0.571	27.870	1.00	15.99		A	N
ANISOU	2554	N	TYR	A	507	2132	1925	2017	22	65	-15	A	N



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ATOM	2556	CA	TYR	A	507	1.965	0.893	27.375	1.00	16.11		A	C
ANISOU	2556	CA	TYR	A	507	2111	1960	2047	10	14	28	A	C
ATOM	2558	CB	TYR	A	507	2.804	-0.394	27.319	1.00	16.03		A	C
ANISOU	2558	CB	TYR	A	507	2078	2006	2005	44	48	63	A	C
ATOM	2561	CG	TYR	A	507	4.287	-0.216	27.036	1.00	16.41		A	C
ANISOU	2561	CG	TYR	A	507	2001	1928	2304	78	28	61	A	C
ATOM	2562	CD1	TYR	A	507	4.874	1.035	26.899	1.00	15.71		A	C
ANISOU	2562	CD1	TYR	A	507	1958	1772	2238	95	-74	32	A	C
ATOM	2564	CE1	TYR	A	507	6.256	1.188	26.625	1.00	18.20		A	C
ANISOU	2564	CE1	TYR	A	507	2382	2113	2419	106	124	138	A	C
ATOM	2566	CZ	TYR	A	507	7.049	0.062	26.502	1.00	21.60		A	C
ANISOU	2566	CZ	TYR	A	507	2658	2565	2981	133	16	126	A	C
ATOM	2567	OH	TYR	A	507	8.395	0.186	26.232	1.00	21.44		A	O
ANISOU	2567	OH	TYR	A	507	2808	2555	2781	138	70	206	A	O
ATOM	2569	CE2	TYR	A	507	6.466	-1.190	26.607	1.00	21.28		A	C
ANISOU	2569	CE2	TYR	A	507	2615	2561	2908	58	65	111	A	C
ATOM	2571	CD2	TYR	A	507	5.113	-1.323	26.882	1.00	18.21		A	C
ANISOU	2571	CD2	TYR	A	507	2420	1966	2530	175	-35	213	A	C
ATOM	2573	C	TYR	A	507	1.858	1.483	25.982	1.00	15.82		A	C
ANISOU	2573	C	TYR	A	507	2098	1941	1972	-1	16	-2	A	C
ATOM	2574	O	TYR	A	507	1.578	0.756	25.041	1.00	16.22		A	O
ANISOU	2574	O	TYR	A	507	2211	1982	1967	-4	41	33	A	O
ATOM	2575	N	ALA	A	508	2.063	2.805	25.872	1.00	15.26		A	N
ANISOU	2575	N	ALA	A	508	2034	1909	1856	-43	23	18	A	N
ATOM	2577	CA	ALA	A	508	2.053	3.513	24.596	1.00	15.39		A	C
ANISOU	2577	CA	ALA	A	508	1965	1962	1919	12	0	6	A	C
ATOM	2579	CB	ALA	A	508	1.309	4.798	24.741	1.00	15.69		A	C
ANISOU	2579	CB	ALA	A	508	2039	2041	1878	11	42	0	A	C
ATOM	2583	C	ALA	A	508	3.458	3.856	24.135	1.00	15.21		A	C
ANISOU	2583	C	ALA	A	508	1917	1965	1897	24	-48	-7	A	C
ATOM	2584	O	ALA	A	508	4.347	4.121	24.957	1.00	16.36		A	O
ANISOU	2584	O	ALA	A	508	1996	2043	2173	54	-97	57	A	O
ATOM	2585	N	LYS	A	509	3.621	3.907	22.816	1.00	15.13		A	N
ANISOU	2585	N	LYS	A	509	1911	1900	1937	36	-8	60	A	N
ATOM	2587	CA	LYS	A	509	4.849	4.341	22.189	1.00	14.90		A	C
ANISOU	2587	CA	LYS	A	509	1847	1930	1885	29	-20	33	A	C
ATOM	2589	CB	LYS	A	509	5.647	3.166	21.611	1.00	15.69		A	C
ANISOU	2589	CB	LYS	A	509	1979	1970	2010	44	38	71	A	C
ATOM	2592	CG	ALYS	A	509	6.331	2.300	22.667	0.50	15.90		A	C
ANISOU	2592	CG	ALYS	A	509	2036	2051	1951	71	-3	9	A	C
ATOM	2593	CG	BLYS	A	509	6.229	2.176	22.598	0.50	16.42		A	C
ANISOU	2593	CG	BLYS	A	509	2092	2100	2045	72	-2	42	A	C
ATOM	2598	CD	ALYS	A	509	7.068	1.123	22.031	0.50	16.13		A	C
ANISOU	2598	CD	ALYS	A	509	2093	2008	2027	45	33	12	A	C
ATOM	2599	CD	BLYS	A	509	6.782	0.968	21.833	0.50	17.51		A	C
ANISOU	2599	CD	BLYS	A	509	2281	2148	2221	35	51	3	A	C
ATOM	2604	CE	ALYS	A	509	7.832	0.299	23.058	0.50	17.05		A	C
ANISOU	2604	CE	ALYS	A	509	2178	2084	2215	67	9	21	A	C
ATOM	2605	CE	BLYS	A	509	7.694	0.114	22.697	0.50	18.67		A	C
ANISOU	2605	CE	BLYS	A	509	2354	2301	2439	34	-69	12	A	C
ATOM	2610	NZ	ALYS	A	509	8.539	-0.848	22.389	0.50	16.82		A	N
ANISOU	2610	NZ	ALYS	A	509	2105	2153	2130	-1	124	-22	A	N
ATOM	2611	NZ	BLYS	A	509	9.141	0.571	22.660	0.50	19.25		A	N
ANISOU	2611	NZ	BLYS	A	509	2376	2391	2548	-3	-29	20	A	N
ATOM	2618	C	LYS	A	509	4.566	5.311	21.047	1.00	14.34		A	C
ANISOU	2618	C	LYS	A	509	1802	1808	1838	65	-29	-1	A	C
ATOM	2619	O	LYS	A	509	3.607	5.168	20.308	1.00	15.81		A	O
ANISOU	2619	O	LYS	A	509	1826	1929	2252	6	-124	-1	A	O
ATOM	2620	N	ILE	A	510	5.439	6.286	20.876	1.00	14.15		A	N
ANISOU	2620	N	ILE	A	510	1794	1773	1809	99	-18	33	A	N
ATOM	2622	CA	ILE	A	510	5.320	7.239	19.780	1.00	13.97		A	C
ANISOU	2622	CA	ILE	A	510	1785	1783	1740	70	37	16	A	C

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ATOM	2624	CB	ILE A 510	6.077	8.534	20.187	1.00	13.91		A	C
ANISOU	2624	CB	ILE A 510	1744	1727	1812	96	9	12	A	C
ATOM	2626	CG1	ILE A 510	5.472	9.139	21.465	1.00	14.89		A	C
ANISOU	2626	CG1	ILE A 510	1864	1903	1889	105	71	-41	A	C
ATOM	2629	CD1	ILE A 510	6.417	9.998	22.213	1.00	15.89		A	C
ANISOU	2629	CD1	ILE A 510	2088	1994	1952	110	35	35	A	C
ATOM	2633	CG2	ILE A 510	6.104	9.575	19.068	1.00	15.14		A	C
ANISOU	2633	CG2	ILE A 510	1949	1871	1932	-40	164	37	A	C
ATOM	2637	C	ILE A 510	5.942	6.655	18.514	1.00	14.32		A	C
ANISOU	2637	C	ILE A 510	1869	1801	1771	68	3	8	A	C
ATOM	2638	O	ILE A 510	7.055	6.136	18.549	1.00	14.94		A	O
ANISOU	2638	O	ILE A 510	2047	1751	1878	56	3	-53	A	O
ATOM	2639	N	SER A 511	5.252	6.809	17.386	1.00	13.90		A	N
ANISOU	2639	N	SER A 511	1798	1745	1736	12	-38	-27	A	N
ATOM	2641	CA	SER A 511	5.743	6.297	16.102	1.00	15.00		A	C
ANISOU	2641	CA	SER A 511	1963	1875	1859	68	33	5	A	C
ATOM	2643	CB	SER A 511	4.932	5.076	15.633	1.00	15.14		A	C
ANISOU	2643	CB	SER A 511	2062	1756	1935	76	92	61	A	C
ATOM	2646	OG	ASER A 511	5.735	4.357	14.689	0.70	15.88		A	O
ANISOU	2646	OG	ASER A 511	2153	1994	1886	131	243	36	A	O
ATOM	2647	OG	BSER A 511	3.614	5.376	15.994	0.30	16.66		A	O
ANISOU	2647	OG	BSER A 511	2068	2041	2221	-43	68	-227	A	O
ATOM	2650	C	SER A 511	5.661	7.406	15.031	1.00	15.71		A	C
ANISOU	2650	C	SER A 511	2207	1876	1883	80	62	9	A	C
ATOM	2651	O	SER A 511	5.419	8.563	15.344	1.00	16.10		A	O
ANISOU	2651	O	SER A 511	2369	1825	1921	45	61	41	A	O
ATOM	2652	N	ASP A 512	5.822	6.996	13.780	1.00	16.81		A	N
ANISOU	2652	N	ASP A 512	2353	2010	2022	75	59	-20	A	N
ATOM	2654	CA	ASP A 512	5.839	7.841	12.581	1.00	16.44		A	C
ANISOU	2654	CA	ASP A 512	2182	2062	2000	32	67	4	A	C
ATOM	2656	CB	ASP A 512	4.463	8.212	12.084	1.00	17.67		A	C
ANISOU	2656	CB	ASP A 512	2383	2157	2171	-45	-18	47	A	C
ATOM	2659	CG	ASP A 512	4.490	8.673	10.635	1.00	19.32		A	C
ANISOU	2659	CG	ASP A 512	2573	2519	2246	-78	15	46	A	C
ATOM	2660	OD1	ASP A 512	5.631	8.875	10.125	1.00	19.18		A	O
ANISOU	2660	OD1	ASP A 512	2557	2499	2231	-198	-121	4	A	O
ATOM	2661	OD2	ASP A 512	3.440	8.810	9.933	1.00	22.44		A	O
ANISOU	2661	OD2	ASP A 512	2775	3018	2730	-99	-101	179	A	O
ATOM	2662	C	ASP A 512	6.703	9.076	12.690	1.00	16.47		A	C
ANISOU	2662	C	ASP A 512	2200	2066	1990	32	27	-22	A	C
ATOM	2663	O	ASP A 512	6.206	10.210	12.850	1.00	16.24		A	O
ANISOU	2663	O	ASP A 512	2193	2036	1939	46	105	95	A	O
ATOM	2664	N	PHE A 513	7.995	8.848	12.499	1.00	16.20		A	N
ANISOU	2664	N	PHE A 513	2174	2013	1968	103	21	-69	A	N
ATOM	2666	CA	PHE A 513	8.994	9.891	12.490	1.00	16.45		A	C
ANISOU	2666	CA	PHE A 513	2108	2161	1979	71	35	15	A	C
ATOM	2668	CB	PHE A 513	10.268	9.379	13.137	1.00	17.38		A	C
ANISOU	2668	CB	PHE A 513	2207	2254	2143	112	81	43	A	C
ATOM	2671	CG	PHE A 513	10.160	9.262	14.632	1.00	15.47		A	C
ANISOU	2671	CG	PHE A 513	1735	2102	2041	210	-82	97	A	C
ATOM	2672	CD1	PHE A 513	9.391	8.279	15.224	1.00	19.38		A	C
ANISOU	2672	CD1	PHE A 513	2505	2561	2295	-22	-18	136	A	C
ATOM	2674	CE1	PHE A 513	9.274	8.238	16.627	1.00	17.20		A	C
ANISOU	2674	CE1	PHE A 513	2080	2296	2158	54	-20	16	A	C
ATOM	2676	CZ	PHE A 513	9.888	9.181	17.396	1.00	16.88		A	C
ANISOU	2676	CZ	PHE A 513	2004	2179	2229	59	-66	178	A	C
ATOM	2678	CE2	PHE A 513	10.600	10.193	16.795	1.00	17.77		A	C
ANISOU	2678	CE2	PHE A 513	2172	2216	2361	26	-15	85	A	C
ATOM	2680	CD2	PHE A 513	10.739	10.221	15.437	1.00	16.97		A	C
ANISOU	2680	CD2	PHE A 513	2223	2004	2218	45	-46	37	A	C
ATOM	2682	C	PHE A 513	9.253	10.434	11.086	1.00	16.51		A	C
ANISOU	2682	C	PHE A 513	2144	2093	2034	44	7	37	A	C

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ATOM	2683	O	PHE	A	513	10.289	11.041	10.839	1.00	16.58	A	O	
ANISOU	2683	O	PHE	A	513	2120	2140	2040	96	-23	67	A	O
ATOM	2684	N	GLY	A	514	8.286	10.257	10.187	1.00	16.51	A	N	
ANISOU	2684	N	GLY	A	514	2152	2108	2011	21	14	-7	A	N
ATOM	2686	CA	GLY	A	514	8.463	10.711	8.809	1.00	16.82	A	C	
ANISOU	2686	CA	GLY	A	514	2210	2099	2082	-18	52	4	A	C
ATOM	2689	C	GLY	A	514	8.704	12.207	8.599	1.00	17.27	A	C	
ANISOU	2689	C	GLY	A	514	2204	2183	2172	-52	71	-4	A	C
ATOM	2690	O	GLY	A	514	9.311	12.580	7.598	1.00	19.81	A	O	
ANISOU	2690	O	GLY	A	514	2782	2511	2233	-24	229	-2	A	O
ATOM	2691	N	LEU	A	515	8.180	13.055	9.477	1.00	16.29	A	N	
ANISOU	2691	N	LEU	A	515	2104	2112	1971	-18	52	-48	A	N
ATOM	2693	CA	LEU	A	515	8.368	14.508	9.394	1.00	16.56	A	C	
ANISOU	2693	CA	LEU	A	515	2092	2134	2064	-27	41	30	A	C
ATOM	2695	CB	LEU	A	515	7.046	15.252	9.634	1.00	17.82	A	C	
ANISOU	2695	CB	LEU	A	515	2347	2215	2208	42	67	14	A	C
ATOM	2698	CG	LEU	A	515	6.000	15.114	8.533	1.00	20.22	A	C	
ANISOU	2698	CG	LEU	A	515	2502	2622	2557	-26	-28	-55	A	C
ATOM	2700	CD1	LEU	A	515	4.706	15.774	8.876	1.00	20.80	A	C	
ANISOU	2700	CD1	LEU	A	515	2472	2825	2605	11	-190	30	A	C
ATOM	2704	CD2	LEU	A	515	6.543	15.737	7.273	1.00	23.61	A	C	
ANISOU	2704	CD2	LEU	A	515	2933	3157	2878	67	-36	188	A	C
ATOM	2708	C	LEU	A	515	9.397	15.019	10.392	1.00	16.34	A	C	
ANISOU	2708	C	LEU	A	515	2068	2083	2054	9	49	27	A	C
ATOM	2709	O	LEU	A	515	9.673	16.203	10.457	1.00	16.72	A	O	
ANISOU	2709	O	LEU	A	515	2060	2084	2208	-54	12	4	A	O
ATOM	2710	N	SER	A	516	9.948	14.124	11.193	1.00	16.21	A	N	
ANISOU	2710	N	SER	A	516	2053	2056	2049	23	31	35	A	N
ATOM	2712	CA	SER	A	516	10.844	14.497	12.274	1.00	15.92	A	C	
ANISOU	2712	CA	SER	A	516	1933	2072	2044	5	40	16	A	C
ATOM	2714	CB	SER	A	516	11.069	13.251	13.156	1.00	15.49	A	C	
ANISOU	2714	CB	SER	A	516	1934	2039	1912	69	-1	29	A	C
ATOM	2717	OG	ASER	A	516	12.029	12.434	12.526	0.70	16.64	A	O	
ANISOU	2717	OG	ASER	A	516	1901	2204	2217	100	109	-11	A	O
ATOM	2718	OG	BSER	A	516	9.906	13.125	13.936	0.30	16.10	A	O	
ANISOU	2718	OG	BSER	A	516	1941	2165	2008	17	20	101	A	O
ATOM	2721	C	SER	A	516	12.152	15.078	11.778	1.00	16.48	A	C	
ANISOU	2721	C	SER	A	516	1969	2227	2062	-5	33	-28	A	C
ATOM	2722	O	SER	A	516	12.615	14.742	10.698	1.00	17.80	A	O	
ANISOU	2722	O	SER	A	516	2082	2570	2108	-88	91	-107	A	O
ATOM	2723	N	LYS	A	517	12.736	15.964	12.572	1.00	16.00	A	N	
ANISOU	2723	N	LYS	A	517	1937	2136	2003	-10	105	-97	A	N
ATOM	2725	CA	LYS	A	517	13.998	16.591	12.219	1.00	16.22	A	C	
ANISOU	2725	CA	LYS	A	517	1985	2129	2050	-18	58	-54	A	C
ATOM	2727	CB	LYS	A	517	13.726	18.011	11.714	1.00	16.89	A	C	
ANISOU	2727	CB	LYS	A	517	1997	2252	2167	11	135	42	A	C
ATOM	2730	CG	LYS	A	517	12.852	18.103	10.507	1.00	18.18	A	C	
ANISOU	2730	CG	LYS	A	517	2209	2351	2348	-8	18	32	A	C
ATOM	2733	CD	LYS	A	517	13.532	17.685	9.227	1.00	21.70	A	C	
ANISOU	2733	CD	LYS	A	517	2709	2896	2640	22	95	0	A	C
ATOM	2736	CE	LYS	A	517	12.552	17.719	8.077	1.00	24.71	A	C	
ANISOU	2736	CE	LYS	A	517	3023	3254	3111	56	-56	-23	A	C
ATOM	2739	NZ	LYS	A	517	13.279	17.513	6.803	1.00	28.10	A	N	
ANISOU	2739	NZ	LYS	A	517	3699	3698	3280	29	97	93	A	N
ATOM	2743	C	LYS	A	517	14.938	16.668	13.412	1.00	16.81	A	C	
ANISOU	2743	C	LYS	A	517	1946	2250	2190	-5	82	-49	A	C
ATOM	2744	O	LYS	A	517	14.518	16.894	14.557	1.00	16.83	A	O	
ANISOU	2744	O	LYS	A	517	1737	2494	2162	-133	170	-16	A	O
ATOM	2745	N	ALA	A	518	16.237	16.523	13.134	1.00	16.54	A	N	
ANISOU	2745	N	ALA	A	518	1826	2214	2244	-43	87	-18	A	N
ATOM	2747	CA	ALA	A	518	17.254	16.725	14.136	1.00	16.38	A	C	
ANISOU	2747	CA	ALA	A	518	1970	2103	2148	12	33	4	A	C

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**Figure 1A – 44**

ATOM	2749	CB	ALA	A	518	18.495	15.929	13.770	1.00	16.85		A	C
ANISOU	2749	CB	ALA	A	518	1903	2206	2290	-32	106	30	A	C
ATOM	2753	C	ALA	A	518	17.596	18.221	14.126	1.00	16.02		A	C
ANISOU	2753	C	ALA	A	518	1730	2146	2211	23	27	15	A	C
ATOM	2754	O	ALA	A	518	17.968	18.779	13.082	1.00	17.99		A	O
ANISOU	2754	O	ALA	A	518	2114	2466	2253	-11	38	5	A	O
ATOM	2755	N	LEU	A	519	17.457	18.881	15.259	1.00	15.38		A	N
ANISOU	2755	N	LEU	A	519	1640	2123	2080	14	-56	57	A	N
ATOM	2757	CA	LEU	A	519	17.730	20.299	15.296	1.00	16.06		A	C
ANISOU	2757	CA	LEU	A	519	1804	2135	2162	9	-3	44	A	C
ATOM	2759	CB	LEU	A	519	17.278	20.903	16.616	1.00	16.19		A	C
ANISOU	2759	CB	LEU	A	519	1884	2156	2111	51	-38	26	A	C
ATOM	2762	CG	LEU	A	519	15.775	20.851	16.860	1.00	17.21		A	C
ANISOU	2762	CG	LEU	A	519	2025	2363	2149	13	44	45	A	C
ATOM	2764	CD1	LEU	A	519	15.430	21.190	18.296	1.00	17.97		A	C
ANISOU	2764	CD1	LEU	A	519	2191	2352	2284	118	5	0	A	C
ATOM	2768	CD2	LEU	A	519	15.087	21.789	15.857	1.00	17.91		A	C
ANISOU	2768	CD2	LEU	A	519	2154	2271	2379	90	23	15	A	C
ATOM	2772	C	LEU	A	519	19.189	20.620	15.109	1.00	15.31		A	C
ANISOU	2772	C	LEU	A	519	1708	2028	2080	36	8	85	A	C
ATOM	2773	O	LEU	A	519	20.047	19.862	15.551	1.00	15.46		A	O
ANISOU	2773	O	LEU	A	519	1463	2243	2167	160	32	58	A	O
ATOM	2774	N	ARG	A	520	19.468	21.715	14.413	1.00	15.53		A	N
ANISOU	2774	N	ARG	A	520	1618	2085	2197	74	-20	115	A	N
ATOM	2776	CA	ARG	A	520	20.849	22.164	14.276	1.00	15.80		A	C
ANISOU	2776	CA	ARG	A	520	1768	2096	2138	-29	17	61	A	C
ATOM	2778	CB	ARG	A	520	20.907	23.438	13.455	1.00	16.96		A	C
ANISOU	2778	CB	ARG	A	520	1944	2217	2283	-23	43	101	A	C
ATOM	2781	CG	ARG	A	520	20.561	23.337	12.040	1.00	19.90		A	C
ANISOU	2781	CG	ARG	A	520	2366	2631	2563	-46	-78	-6	A	C
ATOM	2784	CD	ARG	A	520	20.379	24.718	11.377	1.00	21.14		A	C
ANISOU	2784	CD	ARG	A	520	2560	2667	2802	-80	-65	97	A	C
ATOM	2787	NE	ARG	A	520	21.531	25.605	11.629	1.00	22.06		A	N
ANISOU	2787	NE	ARG	A	520	2802	2903	2674	-183	-191	117	A	N
ATOM	2789	CZ	ARG	A	520	22.362	26.049	10.705	1.00	23.22		A	C
ANISOU	2789	CZ	ARG	A	520	2718	3097	3004	-31	-10	-13	A	C
ATOM	2790	NH1	ARG	A	520	22.231	25.695	9.437	1.00	26.49		A	N
ANISOU	2790	NH1	ARG	A	520	3321	3522	3219	-87	19	32	A	N
ATOM	2793	NH2	ARG	A	520	23.368	26.830	11.060	1.00	23.04		A	N
ANISOU	2793	NH2	ARG	A	520	2926	2877	2949	-107	50	6	A	N
ATOM	2796	C	ARG	A	520	21.427	22.510	15.617	1.00	15.74		A	C
ANISOU	2796	C	ARG	A	520	1743	2113	2122	30	43	70	A	C
ATOM	2797	O	ARG	A	520	20.753	22.924	16.546	1.00	17.10		A	O
ANISOU	2797	O	ARG	A	520	1793	2349	2355	53	116	70	A	O
ATOM	2798	N	ALA	A	521	22.745	22.396	15.732	1.00	15.29		A	N
ANISOU	2798	N	ALA	A	521	1587	2129	2093	7	63	5	A	N
ATOM	2800	CA	ALA	A	521	23.378	22.672	17.000	1.00	14.94		A	C
ANISOU	2800	CA	ALA	A	521	1619	2085	1971	2	66	69	A	C
ATOM	2802	CB	ALA	A	521	24.884	22.322	16.902	1.00	14.75		A	C
ANISOU	2802	CB	ALA	A	521	1483	2079	2041	41	18	93	A	C
ATOM	2806	C	ALA	A	521	23.237	24.089	17.472	1.00	15.63		A	C
ANISOU	2806	C	ALA	A	521	1638	2195	2103	0	-16	35	A	C
ATOM	2807	O	ALA	A	521	23.407	24.347	18.654	1.00	16.73		A	O
ANISOU	2807	O	ALA	A	521	1743	2519	2094	106	13	2	A	O
ATOM	2808	N	ASP	A	522	22.983	25.037	16.571	1.00	16.88		A	N
ANISOU	2808	N	ASP	A	522	1896	2279	2235	-73	-106	31	A	N
ATOM	2810	CA	ASP	A	522	22.918	26.428	16.968	1.00	17.39		A	C
ANISOU	2810	CA	ASP	A	522	2016	2259	2332	-6	-54	65	A	C
ATOM	2812	CB	ASP	A	522	23.770	27.266	15.987	1.00	17.38		A	C
ANISOU	2812	CB	ASP	A	522	1959	2267	2378	-59	-25	81	A	C
ATOM	2815	CG	ASP	A	522	23.291	27.196	14.559	1.00	19.48		A	C
ANISOU	2815	CG	ASP	A	522	2388	2428	2583	-2	-78	140	A	C

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Figure 1A – 45

ATOM	2816	OD1	ASP	A	522	22.467	26.299	14.202	1.00	19.88		A	O
ANISOU	2816	OD1	ASP	A	522	2479	2569	2506	-23	-296	236	A	O
ATOM	2817	OD2	ASP	A	522	23.710	28.035	13.693	1.00	22.65		A	O
ANISOU	2817	OD2	ASP	A	522	2640	2915	3049	-30	129	356	A	O
ATOM	2818	C	ASP	A	522	21.506	27.043	17.066	1.00	17.71		A	C
ANISOU	2818	C	ASP	A	522	2057	2296	2376	-11	-43	4	A	C
ATOM	2819	O	ASP	A	522	21.374	28.230	17.292	1.00	18.68		A	O
ANISOU	2819	O	ASP	A	522	1956	2355	2785	12	-95	59	A	O
ATOM	2820	N	GLU	A	523	20.470	26.232	16.897	1.00	17.63		A	N
ANISOU	2820	N	GLU	A	523	2054	2271	2373	-33	-70	28	A	N
ATOM	2822	CA	GLU	A	523	19.111	26.759	16.927	1.00	18.50		A	C
ANISOU	2822	CA	GLU	A	523	2199	2415	2415	10	11	12	A	C
ATOM	2824	CB	GLU	A	523	18.554	26.909	15.510	1.00	19.41		A	C
ANISOU	2824	CB	GLU	A	523	2248	2562	2564	29	-64	78	A	C
ATOM	2827	CG	GLU	A	523	19.328	27.858	14.587	1.00	22.23		A	C
ANISOU	2827	CG	GLU	A	523	2738	2914	2792	-31	15	180	A	C
ATOM	2830	CD	GLU	A	523	19.249	29.336	14.973	1.00	25.73		A	C
ANISOU	2830	CD	GLU	A	523	3135	3234	3406	7	-47	30	A	C
ATOM	2831	OE1	GLU	A	523	18.532	29.724	15.921	1.00	27.55		A	O
ANISOU	2831	OE1	GLU	A	523	3521	3431	3514	-23	34	79	A	O
ATOM	2832	OE2	GLU	A	523	19.928	30.151	14.304	1.00	28.05		A	O
ANISOU	2832	OE2	GLU	A	523	3541	3344	3772	19	37	316	A	O
ATOM	2833	C	GLU	A	523	18.202	25.804	17.679	1.00	18.24		A	C
ANISOU	2833	C	GLU	A	523	2156	2311	2462	-49	-77	47	A	C
ATOM	2834	O	GLU	A	523	18.440	24.593	17.697	1.00	18.79		A	O
ANISOU	2834	O	GLU	A	523	2113	2413	2611	9	54	47	A	O
ATOM	2835	N	ASN	A	524	17.137	26.343	18.242	1.00	18.20		A	N
ANISOU	2835	N	ASN	A	524	2217	2286	2409	-53	-19	48	A	N
ATOM	2837	CA	ASN	A	524	16.139	25.510	18.928	1.00	18.85		A	C
ANISOU	2837	CA	ASN	A	524	2216	2481	2462	-9	-4	39	A	C
ATOM	2839	CB	ASN	A	524	15.801	26.103	20.296	1.00	20.65		A	C
ANISOU	2839	CB	ASN	A	524	2504	2672	2670	-20	13	-54	A	C
ATOM	2842	CG	ASN	A	524	14.859	27.237	20.224	1.00	23.84		A	C
ANISOU	2842	CG	ASN	A	524	2874	3063	3118	75	-8	-28	A	C
ATOM	2843	OD1	ASN	A	524	14.555	27.748	19.157	1.00	26.34		A	O
ANISOU	2843	OD1	ASN	A	524	3228	3452	3326	212	2	-26	A	O
ATOM	2844	ND2	ASN	A	524	14.359	27.644	21.399	1.00	29.16		A	N
ANISOU	2844	ND2	ASN	A	524	3570	3990	3517	107	144	-265	A	N
ATOM	2847	C	ASN	A	524	14.878	25.251	18.071	1.00	18.11		A	C
ANISOU	2847	C	ASN	A	524	2114	2369	2397	24	26	46	A	C
ATOM	2848	O	ASN	A	524	13.906	24.672	18.536	1.00	19.04		A	O
ANISOU	2848	O	ASN	A	524	2028	2760	2447	22	79	167	A	O
ATOM	2849	N	TYR	A	525	14.974	25.538	16.800	1.00	17.27		A	N
ANISOU	2849	N	TYR	A	525	1875	2348	2336	37	-2	25	A	N
ATOM	2851	CA	TYR	A	525	13.895	25.288	15.867	1.00	17.67		A	C
ANISOU	2851	CA	TYR	A	525	2066	2320	2327	-17	-19	15	A	C
ATOM	2853	CB	TYR	A	525	13.004	26.538	15.727	1.00	18.20		A	C
ANISOU	2853	CB	TYR	A	525	2157	2326	2431	73	64	-37	A	C
ATOM	2856	CG	TYR	A	525	13.700	27.692	15.055	1.00	20.44		A	C
ANISOU	2856	CG	TYR	A	525	2546	2468	2749	35	20	14	A	C
ATOM	2857	CD1	TYR	A	525	14.436	28.608	15.789	1.00	22.87		A	C
ANISOU	2857	CD1	TYR	A	525	2788	2873	3028	15	-75	10	A	C
ATOM	2859	CE1	TYR	A	525	15.107	29.646	15.162	1.00	24.42		A	C
ANISOU	2859	CE1	TYR	A	525	3001	2989	3286	-22	-31	109	A	C
ATOM	2861	CZ	TYR	A	525	15.036	29.778	13.813	1.00	24.99		A	C
ANISOU	2861	CZ	TYR	A	525	3169	3048	3276	-60	18	18	A	C
ATOM	2862	OH	TYR	A	525	15.691	30.838	13.209	1.00	29.38		A	O
ANISOU	2862	OH	TYR	A	525	3823	3578	3763	-231	87	263	A	O
ATOM	2864	CE2	TYR	A	525	14.299	28.910	13.061	1.00	24.99		A	C
ANISOU	2864	CE2	TYR	A	525	3175	3123	3194	-30	39	94	A	C
ATOM	2866	CD2	TYR	A	525	13.635	27.861	13.688	1.00	22.96		A	C
ANISOU	2866	CD2	TYR	A	525	2971	2795	2955	-6	35	2	A	C

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Figure 1A – 46

ATOM	2868	C	TYR	A	525	14.391	24.873	14.507	1.00	17.15		A	C
ANISOU	2868	C	TYR	A	525	1978	2281	2255	-18	4	76	A	C
ATOM	2869	O	TYR	A	525	15.530	25.182	14.128	1.00	17.44		A	O
ANISOU	2869	O	TYR	A	525	1774	2556	2295	-15	-47	56	A	O
ATOM	2870	N	TYR	A	526	13.529	24.167	13.781	1.00	16.55		A	N
ANISOU	2870	N	TYR	A	526	1914	2178	2192	21	-9	39	A	N
ATOM	2872	CA	TYR	A	526	13.712	23.797	12.398	1.00	17.17		A	C
ANISOU	2872	CA	TYR	A	526	2038	2207	2276	-10	44	74	A	C
ATOM	2874	CB	TYR	A	526	13.247	22.349	12.157	1.00	16.83		A	C
ANISOU	2874	CB	TYR	A	526	1940	2196	2256	40	12	78	A	C
ATOM	2877	CG	TYR	A	526	13.073	22.008	10.699	1.00	18.66		A	C
ANISOU	2877	CG	TYR	A	526	2329	2297	2463	-63	82	-64	A	C
ATOM	2878	CD1	TYR	A	526	14.168	21.715	9.900	1.00	22.67		A	C
ANISOU	2878	CD1	TYR	A	526	2712	2936	2963	-51	75	-97	A	C
ATOM	2880	CE1	TYR	A	526	14.014	21.403	8.592	1.00	23.88		A	C
ANISOU	2880	CE1	TYR	A	526	3154	3020	2900	-72	92	-10	A	C
ATOM	2882	CZ	TYR	A	526	12.742	21.353	8.043	1.00	26.06		A	C
ANISOU	2882	CZ	TYR	A	526	3288	3450	3162	28	50	-65	A	C
ATOM	2883	OH	TYR	A	526	12.562	21.017	6.713	1.00	30.25		A	O
ANISOU	2883	OH	TYR	A	526	4300	3855	3336	-77	8	-97	A	O
ATOM	2885	CE2	TYR	A	526	11.641	21.620	8.802	1.00	23.15		A	C
ANISOU	2885	CE2	TYR	A	526	3011	3002	2783	20	-65	31	A	C
ATOM	2887	CD2	TYR	A	526	11.817	21.954	10.133	1.00	20.27		A	C
ANISOU	2887	CD2	TYR	A	526	2637	2510	2554	23	-24	66	A	C
ATOM	2889	C	TYR	A	526	12.837	24.720	11.549	1.00	18.39		A	C
ANISOU	2889	C	TYR	A	526	2138	2465	2383	34	6	71	A	C
ATOM	2890	O	TYR	A	526	11.642	24.933	11.811	1.00	17.69		A	O
ANISOU	2890	O	TYR	A	526	1886	2449	2384	-103	168	202	A	O
ATOM	2891	N	LYS	A	527	13.424	25.277	10.522	1.00	19.96		A	N
ANISOU	2891	N	LYS	A	527	2332	2671	2581	-52	99	94	A	N
ATOM	2893	CA	LYS	A	527	12.690	26.154	9.641	1.00	21.86		A	C
ANISOU	2893	CA	LYS	A	527	2658	2837	2808	8	49	90	A	C
ATOM	2895	CB	LYS	A	527	13.526	27.404	9.350	1.00	23.35		A	C
ANISOU	2895	CB	LYS	A	527	2884	2972	3014	-55	26	47	A	C
ATOM	2898	CG	LYS	A	527	12.998	28.238	8.199	1.00	27.66		A	C
ANISOU	2898	CG	LYS	A	527	3557	3535	3415	9	-13	111	A	C
ATOM	2901	CD	LYS	A	527	11.799	29.034	8.622	1.00	30.64		A	C
ANISOU	2901	CD	LYS	A	527	3745	3905	3990	109	48	59	A	C
ATOM	2904	CE	LYS	A	527	11.381	30.050	7.534	1.00	33.67		A	C
ANISOU	2904	CE	LYS	A	527	4269	4286	4239	64	-15	146	A	C
ATOM	2907	NZ	LYS	A	527	11.218	29.425	6.167	1.00	35.80		A	N
ANISOU	2907	NZ	LYS	A	527	4490	4560	4550	25	-9	-48	A	N
ATOM	2911	C	LYS	A	527	12.392	25.425	8.345	1.00	23.26		A	C
ANISOU	2911	C	LYS	A	527	2885	3014	2937	55	59	40	A	C
ATOM	2912	O	LYS	A	527	13.313	25.006	7.621	1.00	23.72		A	O
ANISOU	2912	O	LYS	A	527	2872	3230	2910	166	149	49	A	O
ATOM	2913	N	ALA	A	528	11.119	25.238	8.028	1.00	23.39		A	N
ANISOU	2913	N	ALA	A	528	2855	3077	2953	80	43	19	A	N
ATOM	2915	CA	ALA	A	528	10.795	24.614	6.759	1.00	25.89		A	C
ANISOU	2915	CA	ALA	A	528	3250	3322	3263	27	15	-11	A	C
ATOM	2917	CB	ALA	A	528	9.422	23.989	6.810	1.00	25.48		A	C
ANISOU	2917	CB	ALA	A	528	3207	3324	3150	24	75	5	A	C
ATOM	2921	C	ALA	A	528	10.878	25.696	5.668	1.00	27.83		A	C
ANISOU	2921	C	ALA	A	528	3490	3588	3494	14	44	62	A	C
ATOM	2922	O	ALA	A	528	10.621	26.874	5.910	1.00	26.46		A	O
ANISOU	2922	O	ALA	A	528	3398	3459	3196	-37	63	187	A	O
ATOM	2923	N	GLN	A	529	11.272	25.306	4.472	1.00	31.56		A	N
ANISOU	2923	N	GLN	A	529	3987	4087	3915	8	23	-30	A	N
ATOM	2925	CA	GLN	A	529	11.410	26.293	3.409	1.00	34.51		A	C
ANISOU	2925	CA	GLN	A	529	4393	4389	4329	0	33	40	A	C
ATOM	2927	CB	GLN	A	529	12.486	25.853	2.427	1.00	35.79		A	C
ANISOU	2927	CB	GLN	A	529	4559	4573	4464	4	68	-7	A	C

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Figure 1A – 47

ATOM	2930	CG	GLN	A	529	13.807	25.536	3.094	1.00	38.59		A	C
ANISOU	2930	CG	GLN	A	529	4814	4972	4876	68	-7	70	A	C
ATOM	2933	CD	GLN	A	529	14.271	26.662	3.998	1.00	42.98		A	C
ANISOU	2933	CD	GLN	A	529	5440	5439	5450	-51	-47	-85	A	C
ATOM	2934	OE1	GLN	A	529	14.342	27.827	3.567	1.00	46.41		A	O
ANISOU	2934	OE1	GLN	A	529	5928	5745	5959	19	0	89	A	O
ATOM	2935	NE2	GLN	A	529	14.585	26.332	5.257	1.00	45.18		A	N
ANISOU	2935	NE2	GLN	A	529	5766	5805	5594	-45	14	67	A	N
ATOM	2938	C	GLN	A	529	10.092	26.502	2.689	1.00	35.92		A	C
ANISOU	2938	C	GLN	A	529	4550	4600	4499	20	0	18	A	C
ATOM	2939	O	GLN	A	529	9.808	27.600	2.203	1.00	36.49		A	O
ANISOU	2939	O	GLN	A	529	4646	4643	4573	-11	56	73	A	O
ATOM	2940	N	THR	A	530	9.295	25.440	2.625	1.00	37.31		A	N
ANISOU	2940	N	THR	A	530	4746	4750	4681	-27	30	51	A	N
ATOM	2942	CA	THR	A	530	7.999	25.476	1.956	1.00	38.51		A	C
ANISOU	2942	CA	THR	A	530	4849	4922	4860	-14	-4	32	A	C
ATOM	2944	CB	THR	A	530	8.081	24.718	0.620	1.00	39.00		A	C
ANISOU	2944	CB	THR	A	530	4918	4985	4914	-1	13	9	A	C
ATOM	2946	OG1	THR	A	530	6.799	24.718	-0.025	1.00	41.93		A	O
ANISOU	2946	OG1	THR	A	530	5198	5452	5281	8	-51	47	A	O
ATOM	2948	CG2	THR	A	530	8.372	23.229	0.846	1.00	39.60		A	C
ANISOU	2948	CG2	THR	A	530	5032	5027	4987	3	-17	-10	A	C
ATOM	2952	C	THR	A	530	6.934	24.826	2.831	1.00	38.66		A	C
ANISOU	2952	C	THR	A	530	4864	4942	4881	-7	10	28	A	C
ATOM	2953	O	THR	A	530	7.255	24.003	3.693	1.00	38.92		A	O
ANISOU	2953	O	THR	A	530	4889	4988	4908	13	-10	59	A	O
ATOM	2954	N	HIS	A	531	5.673	25.180	2.605	1.00	38.56		A	N
ANISOU	2954	N	HIS	A	531	4857	4913	4880	5	-2	53	A	N
ATOM	2956	CA	HIS	A	531	4.570	24.562	3.346	1.00	38.41		A	C
ANISOU	2956	CA	HIS	A	531	4870	4877	4847	2	-3	18	A	C
ATOM	2958	CB	HIS	A	531	3.348	25.490	3.409	1.00	38.73		A	C
ANISOU	2958	CB	HIS	A	531	4903	4923	4889	0	13	37	A	C
ATOM	2961	CG	HIS	A	531	2.182	24.913	4.159	1.00	39.42		A	C
ANISOU	2961	CG	HIS	A	531	4964	5042	4970	-21	-27	48	A	C
ATOM	2962	ND1	HIS	A	531	1.035	25.628	4.421	1.00	41.15		A	N
ANISOU	2962	ND1	HIS	A	531	5165	5220	5248	-36	81	9	A	N
ATOM	2964	CE1	HIS	A	531	0.184	24.867	5.089	1.00	41.17		A	C
ANISOU	2964	CE1	HIS	A	531	5171	5208	5263	4	15	43	A	C
ATOM	2966	NE2	HIS	A	531	0.733	23.681	5.258	1.00	40.60		A	N
ANISOU	2966	NE2	HIS	A	531	5079	5174	5170	10	-43	45	A	N
ATOM	2968	CD2	HIS	A	531	1.984	23.685	4.686	1.00	40.16		A	C
ANISOU	2968	CD2	HIS	A	531	5117	5059	5083	-21	37	38	A	C
ATOM	2970	C	HIS	A	531	4.204	23.271	2.630	1.00	37.96		A	C
ANISOU	2970	C	HIS	A	531	4808	4814	4799	-6	-22	36	A	C
ATOM	2971	O	HIS	A	531	3.568	23.304	1.581	1.00	38.89		A	O
ANISOU	2971	O	HIS	A	531	4963	4980	4832	-22	-62	73	A	O
ATOM	2972	N	GLY	A	532	4.619	22.137	3.180	1.00	36.61		A	N
ANISOU	2972	N	GLY	A	532	4648	4648	4612	-16	0	8	A	N
ATOM	2974	CA	GLY	A	532	4.312	20.851	2.583	1.00	35.45		A	C
ANISOU	2974	CA	GLY	A	532	4473	4522	4471	-7	18	8	A	C
ATOM	2977	C	GLY	A	532	2.957	20.337	3.031	1.00	34.29		A	C
ANISOU	2977	C	GLY	A	532	4382	4360	4285	2	16	-2	A	C
ATOM	2978	O	GLY	A	532	2.120	21.119	3.466	1.00	34.77		A	O
ANISOU	2978	O	GLY	A	532	4417	4467	4327	17	28	50	A	O
ATOM	2979	N	LYS	A	533	2.722	19.036	2.917	1.00	32.36		A	N
ANISOU	2979	N	LYS	A	533	4068	4170	4057	-7	51	15	A	N
ATOM	2981	CA	LYS	A	533	1.435	18.489	3.333	1.00	31.37		A	C
ANISOU	2981	CA	LYS	A	533	4016	3999	3902	1	2	8	A	C
ATOM	2983	CB	LYS	A	533	1.090	17.225	2.580	1.00	32.16		A	C
ANISOU	2983	CB	LYS	A	533	4099	4105	4013	-25	5	-17	A	C
ATOM	2986	CG	LYS	A	533	1.047	17.398	1.067	1.00	33.95		A	C
ANISOU	2986	CG	LYS	A	533	4362	4369	4165	-29	0	-6	A	C

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Figure 1A – 48

ATOM	2989	CD	LYS A 533	0.212	18.640	0.771	0.00	41.78		A	C
ANISOU	2989	CD	LYS A 533	5291	5291	5291	0	0	0	A	C
ATOM	2992	CE	LYS A 533	-0.514	18.395	-0.553	0.00	44.77		A	C
ANISOU	2992	CE	LYS A 533	5670	5670	5670	0	0	0	A	C
ATOM	2995	NZ	LYS A 533	-0.545	19.635	-1.325	0.00	46.73		A	N
ANISOU	2995	NZ	LYS A 533	5918	5918	5918	0	0	0	A	N
ATOM	2999	C	LYS A 533	1.506	18.222	4.818	1.00	29.05		A	C
ANISOU	2999	C	LYS A 533	3689	3701	3644	9	35	-35	A	C
ATOM	3000	O	LYS A 533	2.041	17.202	5.267	1.00	29.31		A	O
ANISOU	3000	O	LYS A 533	3771	3725	3640	-17	76	-71	A	O
ATOM	3001	N	TRP A 534	0.988	19.192	5.559	1.00	26.29		A	N
ANISOU	3001	N	TRP A 534	3301	3429	3256	-25	-39	-22	A	N
ATOM	3003	CA	TRP A 534	1.077	19.215	6.996	1.00	23.70		A	C
ANISOU	3003	CA	TRP A 534	2935	3121	2947	4	59	52	A	C
ATOM	3005	CB	TRP A 534	1.552	20.589	7.416	1.00	23.72		A	C
ANISOU	3005	CB	TRP A 534	2929	3152	2931	-56	24	11	A	C
ATOM	3008	CG	TRP A 534	2.978	20.889	7.049	1.00	23.05		A	C
ANISOU	3008	CG	TRP A 534	2850	3040	2868	-26	-12	12	A	C
ATOM	3009	CD1	TRP A 534	3.910	20.015	6.585	1.00	23.87		A	C
ANISOU	3009	CD1	TRP A 534	3046	3097	2927	-94	63	-27	A	C
ATOM	3011	NE1	TRP A 534	5.111	20.655	6.388	1.00	22.64		A	N
ANISOU	3011	NE1	TRP A 534	2818	3037	2747	-63	3	48	A	N
ATOM	3013	CE2	TRP A 534	4.964	21.974	6.721	1.00	22.32		A	C
ANISOU	3013	CE2	TRP A 534	2806	3020	2653	-17	24	65	A	C
ATOM	3014	CD2	TRP A 534	3.633	22.159	7.143	1.00	21.76		A	C
ANISOU	3014	CD2	TRP A 534	2782	2908	2577	-73	-2	75	A	C
ATOM	3015	CE3	TRP A 534	3.244	23.426	7.580	1.00	22.03		A	C
ANISOU	3015	CE3	TRP A 534	2675	2991	2704	27	15	143	A	C
ATOM	3017	CZ3	TRP A 534	4.170	24.461	7.533	1.00	22.70		A	C
ANISOU	3017	CZ3	TRP A 534	2844	2886	2893	-2	-90	70	A	C
ATOM	3019	CH2	TRP A 534	5.480	24.232	7.092	1.00	23.79		A	C
ANISOU	3019	CH2	TRP A 534	2902	3148	2988	23	25	110	A	C
ATOM	3021	CZ2	TRP A 534	5.890	23.010	6.697	1.00	23.88		A	C
ANISOU	3021	CZ2	TRP A 534	3036	3119	2915	-72	-36	-7	A	C
ATOM	3023	C	TRP A 534	-0.225	18.922	7.718	1.00	21.81		A	C
ANISOU	3023	C	TRP A 534	2698	2873	2714	2	1	-9	A	C
ATOM	3024	O	TRP A 534	-1.309	19.255	7.237	1.00	20.87		A	O
ANISOU	3024	O	TRP A 534	2576	2833	2520	109	43	30	A	O
ATOM	3025	N	PRO A 535	-0.091	18.292	8.881	1.00	19.42		A	N
ANISOU	3025	N	PRO A 535	2372	2558	2446	4	3	-30	A	N
ATOM	3026	CA	PRO A 535	-1.226	18.030	9.790	1.00	19.01		A	C
ANISOU	3026	CA	PRO A 535	2349	2519	2353	-13	34	-27	A	C
ATOM	3028	CB	PRO A 535	-0.679	16.991	10.746	1.00	19.16		A	C
ANISOU	3028	CB	PRO A 535	2393	2464	2423	56	69	-59	A	C
ATOM	3031	CG	PRO A 535	0.824	17.121	10.673	1.00	19.96		A	C
ANISOU	3031	CG	PRO A 535	2410	2606	2565	0	-3	7	A	C
ATOM	3034	CD	PRO A 535	1.190	17.825	9.428	1.00	20.22		A	C
ANISOU	3034	CD	PRO A 535	2510	2620	2549	60	41	-30	A	C
ATOM	3037	C	PRO A 535	-1.560	19.301	10.579	1.00	17.60		A	C
ANISOU	3037	C	PRO A 535	2109	2333	2244	9	29	35	A	C
ATOM	3038	O	PRO A 535	-1.333	19.418	11.788	1.00	16.42		A	O
ANISOU	3038	O	PRO A 535	1783	2381	2075	171	100	102	A	O
ATOM	3039	N	VAL A 536	-2.080	20.273	9.851	1.00	17.54		A	N
ANISOU	3039	N	VAL A 536	2100	2373	2192	-23	74	12	A	N
ATOM	3041	CA	VAL A 536	-2.266	21.601	10.343	1.00	17.13		A	C
ANISOU	3041	CA	VAL A 536	2109	2236	2162	-62	24	46	A	C
ATOM	3043	CB	VAL A 536	-2.779	22.476	9.170	1.00	18.56		A	C
ANISOU	3043	CB	VAL A 536	2333	2419	2299	-29	42	39	A	C
ATOM	3045	CG1AVAL	A 536	-1.789	22.616	8.002	0.60	18.83		A	C
ANISOU	3045	CG1AVAL	A 536	2333	2470	2351	-33	117	-9	A	C
ATOM	3046	CG1BVAL	A 536	-3.802	23.492	9.603	0.40	18.63		A	C
ANISOU	3046	CG1BVAL	A 536	2434	2327	2316	-50	9	37	A	C



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ATOM	3053	CG2AVAL	A	536	-4.255	22.497	8.899	0.60	17.32		A	C	
ANISOU	3053	CG2AVAL	A	536	2257	2271	2051	-59	19	-8	A	C	
ATOM	3054	CG2BVAL	A	536	-1.610	23.072	8.384	0.40	18.60		A	C	
ANISOU	3054	CG2BVAL	A	536	2315	2449	2300	-46	41	-35	A	C	
ATOM	3061	C	VAL	A	536	-3.106	21.718	11.615	1.00	14.55	A	C	
ANISOU	3061	C	VAL	A	536	1772	1845	1909	27	-1	-9	A	C
ATOM	3062	O	VAL	A	536	-2.863	22.605	12.434	1.00	14.52	A	O	
ANISOU	3062	O	VAL	A	536	1714	2036	1764	117	-145	127	A	O
ATOM	3063	N	LYS	A	537	-4.098	20.833	11.794	1.00	13.86	A	N	
ANISOU	3063	N	LYS	A	537	1755	1815	1696	30	-71	-20	A	N
ATOM	3065	CA	LYS	A	537	-4.918	20.909	13.000	1.00	13.56	A	C	
ANISOU	3065	CA	LYS	A	537	1596	1816	1740	60	-39	24	A	C
ATOM	3067	CB	LYS	A	537	-6.165	20.038	12.876	1.00	14.21	A	C	
ANISOU	3067	CB	LYS	A	537	1751	1840	1806	16	-33	75	A	C
ATOM	3070	CG	LYS	A	537	-7.165	20.661	11.903	1.00	15.10	A	C	
ANISOU	3070	CG	LYS	A	537	1820	2097	1818	101	-5	55	A	C
ATOM	3073	CD	LYS	A	537	-8.365	19.818	11.727	1.00	16.89	A	C	
ANISOU	3073	CD	LYS	A	537	2046	2245	2124	-12	-9	-50	A	C
ATOM	3076	CE	LYS	A	537	-9.414	20.551	10.903	1.00	19.41	A	C	
ANISOU	3076	CE	LYS	A	537	2295	2631	2447	-28	-35	137	A	C
ATOM	3079	NZ	LYS	A	537	-10.597	19.623	10.675	1.00	23.77	A	N	
ANISOU	3079	NZ	LYS	A	537	2725	3182	3123	-255	-214	32	A	N
ATOM	3083	C	LYS	A	537	-4.128	20.569	14.272	1.00	13.85	A	C	
ANISOU	3083	C	LYS	A	537	1666	1897	1699	61	-46	4	A	C
ATOM	3084	O	LYS	A	537	-4.599	20.824	15.379	1.00	14.39	A	O	
ANISOU	3084	O	LYS	A	537	1576	2110	1779	118	-102	-22	A	O
ATOM	3085	N	TRP	A	538	-2.937	19.995	14.105	1.00	13.24	A	N	
ANISOU	3085	N	TRP	A	538	1594	1847	1587	92	-47	-49	A	N
ATOM	3087	CA	TRP	A	538	-2.075	19.699	15.260	1.00	12.67	A	C	
ANISOU	3087	CA	TRP	A	538	1521	1700	1592	72	-55	33	A	C
ATOM	3089	CB	TRP	A	538	-1.514	18.267	15.129	1.00	13.12	A	C	
ANISOU	3089	CB	TRP	A	538	1518	1703	1761	29	-104	101	A	C
ATOM	3092	CG	TRP	A	538	-2.526	17.198	15.416	1.00	12.33	A	C	
ANISOU	3092	CG	TRP	A	538	1485	1576	1623	0	-33	-33	A	C
ATOM	3093	CD1	TRP	A	538	-2.663	16.510	16.570	1.00	14.35	A	C	
ANISOU	3093	CD1	TRP	A	538	1747	1832	1871	-94	-54	21	A	C
ATOM	3095	NE1	TRP	A	538	-3.726	15.646	16.497	1.00	13.50	A	N	
ANISOU	3095	NE1	TRP	A	538	1468	1789	1872	99	34	-54	A	N
ATOM	3097	CE2	TRP	A	538	-4.277	15.748	15.253	1.00	13.38	A	C	
ANISOU	3097	CE2	TRP	A	538	1510	1796	1775	-26	77	-108	A	C
ATOM	3098	CD2	TRP	A	538	-3.554	16.734	14.551	1.00	13.26	A	C	
ANISOU	3098	CD2	TRP	A	538	1536	1717	1783	83	-5	-16	A	C
ATOM	3099	CE3	TRP	A	538	-3.915	17.013	13.238	1.00	13.92	A	C	
ANISOU	3099	CE3	TRP	A	538	1650	1784	1854	-176	45	184	A	C
ATOM	3101	CZ3	TRP	A	538	-4.969	16.329	12.686	1.00	15.45	A	C	
ANISOU	3101	CZ3	TRP	A	538	1800	2079	1991	20	-142	44	A	C
ATOM	3103	CH2	TRP	A	538	-5.680	15.372	13.411	1.00	15.75	A	C	
ANISOU	3103	CH2	TRP	A	538	2009	2002	1972	-74	-152	-17	A	C
ATOM	3105	CZ2	TRP	A	538	-5.356	15.060	14.693	1.00	14.55	A	C	
ANISOU	3105	CZ2	TRP	A	538	1633	2009	1884	-127	56	-58	A	C
ATOM	3107	C	TRP	A	538	-0.916	20.688	15.447	1.00	13.57	A	C	
ANISOU	3107	C	TRP	A	538	1589	1829	1735	85	-28	92	A	C
ATOM	3108	O	TRP	A	538	-0.132	20.542	16.394	1.00	14.48	A	O	
ANISOU	3108	O	TRP	A	538	1664	1981	1855	13	-78	7	A	O
ATOM	3109	N	TYR	A	539	-0.837	21.694	14.573	1.00	13.35	A	N	
ANISOU	3109	N	TYR	A	539	1498	1669	1903	-55	60	89	A	N
ATOM	3111	CA	TYR	A	539	0.302	22.609	14.516	1.00	14.33	A	C	
ANISOU	3111	CA	TYR	A	539	1744	1825	1875	-31	-43	77	A	C
ATOM	3113	CB	TYR	A	539	0.687	22.860	13.073	1.00	14.42	A	C	
ANISOU	3113	CB	TYR	A	539	1737	1796	1946	-78	4	54	A	C
ATOM	3116	CG	TYR	A	539	1.565	21.800	12.443	1.00	15.18	A	C	
ANISOU	3116	CG	TYR	A	539	1877	1930	1960	-38	5	28	A	C

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ATOM	3117	CD1	TYR	A	539	1.928	20.658	13.134	1.00	16.80		A	C
ANISOU	3117	CD1	TYR	A	539	2128	2022	2231	197	-29	33	A	C
ATOM	3119	CE1	TYR	A	539	2.789	19.708	12.550	1.00	17.20		A	C
ANISOU	3119	CE1	TYR	A	539	2162	2285	2088	96	141	-102	A	C
ATOM	3121	CZ	TYR	A	539	3.251	19.937	11.273	1.00	17.43		A	C
ANISOU	3121	CZ	TYR	A	539	2258	2220	2143	125	77	13	A	C
ATOM	3122	OH	TYR	A	539	4.090	19.044	10.675	1.00	16.94		A	O
ANISOU	3122	OH	TYR	A	539	2004	2314	2116	204	77	58	A	O
ATOM	3124	CE2	TYR	A	539	2.904	21.070	10.604	1.00	16.51		A	C
ANISOU	3124	CE2	TYR	A	539	2105	2170	1996	111	100	11	A	C
ATOM	3126	CD2	TYR	A	539	2.074	21.976	11.188	1.00	16.23		A	C
ANISOU	3126	CD2	TYR	A	539	2056	2084	2024	96	-32	102	A	C
ATOM	3128	C	TYR	A	539	0.066	23.927	15.251	1.00	14.09		A	C
ANISOU	3128	C	TYR	A	539	1704	1799	1848	8	-22	40	A	C
ATOM	3129	O	TYR	A	539	-1.025	24.543	15.184	1.00	15.96		A	O
ANISOU	3129	O	TYR	A	539	1771	2159	2134	111	-51	-37	A	O
ATOM	3130	N	ALA	A	540	1.126	24.398	15.907	1.00	14.28		A	N
ANISOU	3130	N	ALA	A	540	1713	1865	1848	14	10	45	A	N
ATOM	3132	CA	ALA	A	540	1.117	25.661	16.616	1.00	14.45		A	C
ANISOU	3132	CA	ALA	A	540	1835	1824	1827	16	18	76	A	C
ATOM	3134	CB	ALA	A	540	2.297	25.725	17.565	1.00	14.70		A	C
ANISOU	3134	CB	ALA	A	540	1855	1806	1922	-18	-21	31	A	C
ATOM	3138	C	ALA	A	540	1.140	26.846	15.636	1.00	14.61		A	C
ANISOU	3138	C	ALA	A	540	1848	1845	1858	62	46	68	A	C
ATOM	3139	O	ALA	A	540	1.497	26.696	14.482	1.00	14.39		A	O
ANISOU	3139	O	ALA	A	540	1763	1845	1859	48	46	163	A	O
ATOM	3140	N	PRO	A	541	0.680	27.997	16.089	1.00	15.21		A	N
ANISOU	3140	N	PRO	A	541	1970	1901	1907	51	82	42	A	N
ATOM	3141	CA	PRO	A	541	0.635	29.176	15.226	1.00	15.70		A	C
ANISOU	3141	CA	PRO	A	541	1981	1979	2004	62	80	68	A	C
ATOM	3143	CB	PRO	A	541	0.142	30.275	16.166	1.00	16.44		A	C
ANISOU	3143	CB	PRO	A	541	2107	2011	2129	66	87	81	A	C
ATOM	3146	CG	PRO	A	541	-0.654	29.523	17.201	1.00	16.57		A	C
ANISOU	3146	CG	PRO	A	541	2079	2109	2106	137	97	46	A	C
ATOM	3149	CD	PRO	A	541	0.094	28.242	17.434	1.00	15.35		A	C
ANISOU	3149	CD	PRO	A	541	1930	1912	1990	104	129	88	A	C
ATOM	3152	C	PRO	A	541	1.968	29.514	14.586	1.00	16.46		A	C
ANISOU	3152	C	PRO	A	541	2099	2081	2073	98	85	74	A	C
ATOM	3153	O	PRO	A	541	2.003	29.901	13.411	1.00	17.24		A	O
ANISOU	3153	O	PRO	A	541	2217	2275	2058	167	97	273	A	O
ATOM	3154	N	GLU	A	542	3.062	29.343	15.307	1.00	15.42		A	N
ANISOU	3154	N	GLU	A	542	1953	1925	1980	9	37	133	A	N
ATOM	3156	CA	GLU	A	542	4.372	29.681	14.710	1.00	16.70		A	C
ANISOU	3156	CA	GLU	A	542	2095	2113	2135	0	65	71	A	C
ATOM	3158	CB	GLU	A	542	5.478	29.714	15.757	1.00	17.09		A	C
ANISOU	3158	CB	GLU	A	542	2118	2179	2196	-40	119	53	A	C
ATOM	3161	CG	GLU	A	542	5.830	28.371	16.339	1.00	17.33		A	C
ANISOU	3161	CG	GLU	A	542	2141	2213	2228	9	-11	65	A	C
ATOM	3164	CD	GLU	A	542	5.040	27.987	17.578	1.00	16.39		A	C
ANISOU	3164	CD	GLU	A	542	2095	1943	2188	-6	56	-49	A	C
ATOM	3165	OE1	GLU	A	542	4.041	28.665	17.937	1.00	16.71		A	O
ANISOU	3165	OE1	GLU	A	542	2141	1993	2214	-5	208	47	A	O
ATOM	3166	OE2	GLU	A	542	5.423	26.947	18.174	1.00	14.95		A	O
ANISOU	3166	OE2	GLU	A	542	1535	2171	1972	114	42	96	A	O
ATOM	3167	C	GLU	A	542	4.735	28.764	13.547	1.00	16.70		A	C
ANISOU	3167	C	GLU	A	542	2042	2170	2133	6	5	72	A	C
ATOM	3168	O	GLU	A	542	5.490	29.126	12.648	1.00	16.98		A	O
ANISOU	3168	O	GLU	A	542	2121	2220	2108	-49	21	186	A	O
ATOM	3169	N	CYS	A	543	4.214	27.556	13.579	1.00	16.05		A	N
ANISOU	3169	N	CYS	A	543	1959	2044	2095	-2	28	68	A	N
ATOM	3171	CA	CYS	A	543	4.443	26.623	12.497	1.00	15.51		A	C
ANISOU	3171	CA	CYS	A	543	1796	2097	2001	10	24	26	A	C

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ATOM	3173	CB	CYS	A	543	3.944	25.224	12.874	1.00	15.84		A	C
ANISOU	3173	CB	CYS	A	543	1787	2106	2126	88	-25	26	A	C
ATOM	3176	SG	CYS	A	543	4.561	24.579	14.420	1.00	16.92		A	S
ANISOU	3176	SG	CYS	A	543	1961	2232	2235	230	106	172	A	S
ATOM	3177	C	CYS	A	543	3.746	27.101	11.233	1.00	16.91		A	C
ANISOU	3177	C	CYS	A	543	2072	2249	2103	64	41	40	A	C
ATOM	3178	O	CYS	A	543	4.311	27.088	10.140	1.00	17.45		A	O
ANISOU	3178	O	CYS	A	543	2158	2467	2004	67	30	162	A	O
ATOM	3179	N	ILE	A	544	2.499	27.488	11.398	1.00	17.27		A	N
ANISOU	3179	N	ILE	A	544	2050	2382	2128	67	29	38	A	N
ATOM	3181	CA	ILE	A	544	1.671	27.896	10.282	1.00	18.64		A	C
ANISOU	3181	CA	ILE	A	544	2242	2515	2325	115	8	38	A	C
ATOM	3183	CB	ILE	A	544	0.191	27.977	10.746	1.00	19.22		A	C
ANISOU	3183	CB	ILE	A	544	2268	2583	2452	97	21	42	A	C
ATOM	3185	CG1	ILE	A	544	-0.331	26.629	11.252	1.00	20.83		A	C
ANISOU	3185	CG1	ILE	A	544	2390	2785	2737	2	26	27	A	C
ATOM	3188	CD1	ILE	A	544	-0.274	25.556	10.276	1.00	23.31		A	C
ANISOU	3188	CD1	ILE	A	544	2934	3027	2895	-9	-45	50	A	C
ATOM	3192	CG2	ILE	A	544	-0.687	28.508	9.612	1.00	20.73		A	C
ANISOU	3192	CG2	ILE	A	544	2610	2702	2563	96	-63	88	A	C
ATOM	3196	C	ILE	A	544	2.102	29.246	9.747	1.00	19.05		A	C
ANISOU	3196	C	ILE	A	544	2324	2525	2386	169	16	67	A	C
ATOM	3197	O	ILE	A	544	2.181	29.454	8.509	1.00	20.61		A	O
ANISOU	3197	O	ILE	A	544	2727	2735	2367	295	69	136	A	O
ATOM	3198	N	ASN	A	545	2.403	30.167	10.647	1.00	19.33		A	N
ANISOU	3198	N	ASN	A	545	2411	2469	2463	81	40	126	A	N
ATOM	3200	CA	ASN	A	545	2.727	31.551	10.268	1.00	20.28		A	C
ANISOU	3200	CA	ASN	A	545	2565	2556	2585	54	27	140	A	C
ATOM	3202	CB	ASN	A	545	2.407	32.495	11.414	1.00	20.76		A	C
ANISOU	3202	CB	ASN	A	545	2637	2568	2681	71	-6	112	A	C
ATOM	3205	CG	ASN	A	545	0.934	32.576	11.709	1.00	22.52		A	C
ANISOU	3205	CG	ASN	A	545	2698	2894	2964	119	34	44	A	C
ATOM	3206	OD1	ASN	A	545	0.522	32.778	12.868	1.00	27.07		A	O
ANISOU	3206	OD1	ASN	A	545	3281	3519	3482	257	131	146	A	O
ATOM	3207	ND2	ASN	A	545	0.131	32.393	10.685	1.00	23.96		A	N
ANISOU	3207	ND2	ASN	A	545	2709	3320	3074	265	70	-77	A	N
ATOM	3210	C	ASN	A	545	4.166	31.786	9.873	1.00	19.86		A	C
ANISOU	3210	C	ASN	A	545	2493	2478	2573	76	91	227	A	C
ATOM	3211	O	ASN	A	545	4.448	32.669	9.020	1.00	21.97		A	O
ANISOU	3211	O	ASN	A	545	2860	2694	2790	158	209	383	A	O
ATOM	3212	N	TYR	A	546	5.088	31.033	10.471	1.00	19.53		A	N
ANISOU	3212	N	TYR	A	546	2403	2529	2487	65	128	174	A	N
ATOM	3214	CA	TYR	A	546	6.517	31.252	10.226	1.00	19.24		A	C
ANISOU	3214	CA	TYR	A	546	2402	2411	2495	3	110	137	A	C
ATOM	3216	CB	TYR	A	546	7.165	31.861	11.456	1.00	19.14		A	C
ANISOU	3216	CB	TYR	A	546	2434	2362	2473	-51	166	201	A	C
ATOM	3219	CG	TYR	A	546	6.580	33.214	11.767	1.00	23.74		A	C
ANISOU	3219	CG	TYR	A	546	3130	2722	3168	81	172	-1	A	C
ATOM	3220	CD1	TYR	A	546	6.939	34.326	11.006	1.00	27.82		A	C
ANISOU	3220	CD1	TYR	A	546	3666	3251	3653	-15	233	184	A	C
ATOM	3222	CE1	TYR	A	546	6.373	35.568	11.246	1.00	29.28		A	C
ANISOU	3222	CE1	TYR	A	546	3898	3447	3781	88	102	-15	A	C
ATOM	3224	CZ	TYR	A	546	5.431	35.705	12.235	1.00	29.56		A	C
ANISOU	3224	CZ	TYR	A	546	3797	3530	3902	12	129	63	A	C
ATOM	3225	OH	TYR	A	546	4.889	36.964	12.486	1.00	32.82		A	O
ANISOU	3225	OH	TYR	A	546	4256	3719	4495	144	234	-101	A	O
ATOM	3227	CE2	TYR	A	546	5.054	34.614	12.995	1.00	26.10		A	C
ANISOU	3227	CE2	TYR	A	546	3370	3129	3414	84	152	-101	A	C
ATOM	3229	CD2	TYR	A	546	5.637	33.376	12.754	1.00	23.89		A	C
ANISOU	3229	CD2	TYR	A	546	3034	2802	3239	-124	181	76	A	C
ATOM	3231	C	TYR	A	546	7.303	30.013	9.821	1.00	18.61		A	C
ANISOU	3231	C	TYR	A	546	2310	2396	2363	25	62	151	A	C

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ATOM	3232	O	TYR A 546	8.493	30.107	9.627	1.00	19.39		A	O
ANISOU	3232	O	TYR A 546	2285	2466	2615	-58	199	211	A	O
ATOM	3233	N	TYR A 547	6.649	28.873	9.710	1.00	17.93		A	N
ANISOU	3233	N	TYR A 547	2225	2334	2253	41	49	134	A	N
ATOM	3235	CA	TYR A 547	7.282	27.618	9.317	1.00	18.52		A	C
ANISOU	3235	CA	TYR A 547	2311	2441	2285	14	113	64	A	C
ATOM	3237	CB	TYR A 547	7.893	27.731	7.908	1.00	19.52		A	C
ANISOU	3237	CB	TYR A 547	2414	2617	2383	41	169	114	A	C
ATOM	3240	CG	TYR A 547	6.940	28.052	6.806	1.00	22.56		A	C
ANISOU	3240	CG	TYR A 547	2809	2973	2786	59	35	108	A	C
ATOM	3241	CD1	TYR A 547	5.577	28.042	6.998	1.00	25.10		A	C
ANISOU	3241	CD1	TYR A 547	3048	3267	3221	-20	46	103	A	C
ATOM	3243	CE1	TYR A 547	4.715	28.352	5.974	1.00	27.68		A	C
ANISOU	3243	CE1	TYR A 547	3409	3634	3474	125	-15	2	A	C
ATOM	3245	CZ	TYR A 547	5.217	28.663	4.731	1.00	30.88		A	C
ANISOU	3245	CZ	TYR A 547	3797	4103	3830	22	54	122	A	C
ATOM	3246	OH	TYR A 547	4.360	28.958	3.698	1.00	35.32		A	O
ANISOU	3246	OH	TYR A 547	4495	4842	4081	72	-134	147	A	O
ATOM	3248	CE2	TYR A 547	6.566	28.674	4.517	1.00	29.53		A	C
ANISOU	3248	CE2	TYR A 547	3691	4019	3507	52	-5	125	A	C
ATOM	3250	CD2	TYR A 547	7.418	28.368	5.545	1.00	27.26		A	C
ANISOU	3250	CD2	TYR A 547	3418	3757	3181	-12	147	83	A	C
ATOM	3252	C	TYR A 547	8.352	27.193	10.308	1.00	18.06		A	C
ANISOU	3252	C	TYR A 547	2276	2314	2272	39	127	118	A	C
ATOM	3253	O	TYR A 547	9.321	26.501	9.930	1.00	17.59		A	O
ANISOU	3253	O	TYR A 547	2110	2360	2213	99	234	182	A	O
ATOM	3254	N	LYS A 548	8.166	27.571	11.573	1.00	16.63		A	N
ANISOU	3254	N	LYS A 548	2028	2132	2158	28	124	72	A	N
ATOM	3256	CA	LYS A 548	9.145	27.277	12.630	1.00	17.24		A	C
ANISOU	3256	CA	LYS A 548	2136	2239	2174	-37	112	138	A	C
ATOM	3258	CB	LYS A 548	9.473	28.512	13.448	1.00	18.66		A	C
ANISOU	3258	CB	LYS A 548	2349	2366	2376	78	105	136	A	C
ATOM	3261	CG	LYS A 548	10.297	29.548	12.679	1.00	21.31		A	C
ANISOU	3261	CG	LYS A 548	2615	2740	2740	-47	22	204	A	C
ATOM	3264	CD	LYS A 548	10.513	30.812	13.454	1.00	24.06		A	C
ANISOU	3264	CD	LYS A 548	3063	2991	3089	-19	9	63	A	C
ATOM	3267	CE	LYS A 548	11.396	30.613	14.680	1.00	26.24		A	C
ANISOU	3267	CE	LYS A 548	3325	3350	3292	49	-59	30	A	C
ATOM	3270	NZ	LYS A 548	11.590	31.879	15.473	1.00	28.92		A	N
ANISOU	3270	NZ	LYS A 548	3637	3548	3803	40	-60	-102	A	N
ATOM	3274	C	LYS A 548	8.650	26.165	13.544	1.00	16.61		A	C
ANISOU	3274	C	LYS A 548	2085	2099	2125	48	110	124	A	C
ATOM	3275	O	LYS A 548	7.564	26.259	14.093	1.00	16.85		A	O
ANISOU	3275	O	LYS A 548	2067	2073	2262	136	177	170	A	O
ATOM	3276	N	PHE A 549	9.492	25.147	13.716	1.00	15.25		A	N
ANISOU	3276	N	PHE A 549	1828	1968	1998	14	72	87	A	N
ATOM	3278	CA	PHE A 549	9.159	23.948	14.483	1.00	15.17		A	C
ANISOU	3278	CA	PHE A 549	1806	2000	1956	-20	48	63	A	C
ATOM	3280	CB	PHE A 549	9.107	22.733	13.564	1.00	15.51		A	C
ANISOU	3280	CB	PHE A 549	1838	2035	2019	-5	26	97	A	C
ATOM	3283	CG	PHE A 549	8.032	22.828	12.511	1.00	15.30		A	C
ANISOU	3283	CG	PHE A 549	1773	2066	1971	22	21	85	A	C
ATOM	3284	CD1	PHE A 549	8.288	23.458	11.306	1.00	15.37		A	C
ANISOU	3284	CD1	PHE A 549	1811	2023	2004	-52	0	74	A	C
ATOM	3286	CE1	PHE A 549	7.314	23.580	10.341	1.00	15.75		A	C
ANISOU	3286	CE1	PHE A 549	1937	2017	2028	39	-14	-33	A	C
ATOM	3288	CZ	PHE A 549	6.073	23.035	10.568	1.00	16.53		A	C
ANISOU	3288	CZ	PHE A 549	1944	2227	2110	81	110	8	A	C
ATOM	3290	CE2	PHE A 549	5.809	22.394	11.760	1.00	16.94		A	C
ANISOU	3290	CE2	PHE A 549	2044	2251	2139	-65	-61	57	A	C
ATOM	3292	CD2	PHE A 549	6.782	22.300	12.728	1.00	15.67		A	C
ANISOU	3292	CD2	PHE A 549	1879	1963	2110	38	-60	97	A	C

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ATOM	3294	C	PHE A 549	10.154	23.694	15.598	1.00	15.41		A	C
ANISOU	3294	C	PHE A 549	1818	2057	1978	59	47	59	A	C
ATOM	3295	O	PHE A 549	11.341	23.471	15.343	1.00	16.52		A	O
ANISOU	3295	O	PHE A 549	1693	2385	2196	55	39	145	A	O
ATOM	3296	N	SER A 550	9.679	23.712	16.828	1.00	14.73		A	N
ANISOU	3296	N	SER A 550	1641	2030	1923	63	47	113	A	N
ATOM	3298	CA	SER A 550	10.525	23.481	17.993	1.00	14.70		A	C
ANISOU	3298	CA	SER A 550	1646	2053	1885	78	42	56	A	C
ATOM	3300	CB	SER A 550	10.644	24.760	18.794	1.00	15.51		A	C
ANISOU	3300	CB	SER A 550	1803	2075	2015	-22	28	194	A	C
ATOM	3303	OG	SER A 550	9.354	25.199	19.249	1.00	18.11		A	O
ANISOU	3303	OG	SER A 550	2066	2261	2553	131	179	35	A	O
ATOM	3305	C	SER A 550	9.891	22.426	18.871	1.00	13.72		A	C
ANISOU	3305	C	SER A 550	1613	1826	1772	71	-31	-6	A	C
ATOM	3306	O	SER A 550	8.772	21.954	18.601	1.00	13.57		A	O
ANISOU	3306	O	SER A 550	1352	1968	1834	148	-3	-6	A	O
ATOM	3307	N	SER A 551	10.569	22.055	19.957	1.00	14.11		A	N
ANISOU	3307	N	SER A 551	1594	2002	1762	113	-34	28	A	N
ATOM	3309	CA	SER A 551	9.913	21.189	20.920	1.00	14.15		A	C
ANISOU	3309	CA	SER A 551	1644	1929	1801	39	-66	51	A	C
ATOM	3311	CB	SER A 551	10.846	20.765	22.054	1.00	14.82		A	C
ANISOU	3311	CB	SER A 551	1760	2062	1809	74	-43	98	A	C
ATOM	3314	OG	SER A 551	11.839	19.888	21.506	1.00	15.10		A	O
ANISOU	3314	OG	SER A 551	1553	2207	1975	99	0	-11	A	O
ATOM	3316	C	SER A 551	8.667	21.847	21.466	1.00	14.38		A	C
ANISOU	3316	C	SER A 551	1748	1899	1815	19	-46	45	A	C
ATOM	3317	O	SER A 551	7.680	21.148	21.748	1.00	14.51		A	O
ANISOU	3317	O	SER A 551	1728	1921	1863	-57	0	69	A	O
ATOM	3318	N	LYS A 552	8.669	23.177	21.619	1.00	14.30		A	N
ANISOU	3318	N	LYS A 552	1638	1822	1974	8	33	-12	A	N
ATOM	3320	CA	LYS A 552	7.437	23.875	22.066	1.00	15.23		A	C
ANISOU	3320	CA	LYS A 552	1823	1960	2000	68	-21	11	A	C
ATOM	3322	CB	LYS A 552	7.665	25.387	22.266	1.00	16.28		A	C
ANISOU	3322	CB	LYS A 552	1905	2094	2183	32	4	42	A	C
ATOM	3325	CG	LYS A 552	8.650	25.750	23.343	1.00	20.78		A	C
ANISOU	3325	CG	LYS A 552	2526	2698	2670	-21	-105	-112	A	C
ATOM	3328	CD	LYS A 552	8.130	25.620	24.694	1.00	21.47		A	C
ANISOU	3328	CD	LYS A 552	2457	2933	2767	99	-95	63	A	C
ATOM	3331	CE	LYS A 552	9.090	26.245	25.752	1.00	21.81		A	C
ANISOU	3331	CE	LYS A 552	2587	2823	2875	-21	-74	-125	A	C
ATOM	3334	NZ	LYS A 552	9.006	27.711	26.072	1.00	21.76		A	N
ANISOU	3334	NZ	LYS A 552	2501	2833	2934	-19	-9	19	A	N
ATOM	3338	C	LYS A 552	6.299	23.661	21.059	1.00	13.53		A	C
ANISOU	3338	C	LYS A 552	1636	1663	1840	28	24	63	A	C
ATOM	3339	O	LYS A 552	5.129	23.603	21.465	1.00	13.35		A	O
ANISOU	3339	O	LYS A 552	1472	1797	1801	185	72	157	A	O
ATOM	3340	N	SER A 553	6.604	23.635	19.758	1.00	13.10		A	N
ANISOU	3340	N	SER A 553	1598	1561	1820	1	-10	82	A	N
ATOM	3342	CA	SER A 553	5.575	23.334	18.759	1.00	13.62		A	C
ANISOU	3342	CA	SER A 553	1610	1767	1796	28	-2	98	A	C
ATOM	3344	CB	SER A 553	6.087	23.512	17.316	1.00	15.50		A	C
ANISOU	3344	CB	SER A 553	2085	1936	1866	-54	-166	170	A	C
ATOM	3347	OG	SER A 553	6.848	24.716	17.238	1.00	20.01		A	O
ANISOU	3347	OG	SER A 553	2472	2452	2676	-89	0	97	A	O
ATOM	3349	C	SER A 553	5.029	21.927	19.007	1.00	12.87		A	C
ANISOU	3349	C	SER A 553	1530	1704	1653	22	-96	57	A	C
ATOM	3350	O	SER A 553	3.828	21.679	18.896	1.00	13.18		A	O
ANISOU	3350	O	SER A 553	1305	1894	1807	70	64	167	A	O
ATOM	3351	N	ASP A 554	5.896	20.978	19.330	1.00	12.17		A	N
ANISOU	3351	N	ASP A 554	1326	1625	1671	38	-15	88	A	N
ATOM	3353	CA	ASP A 554	5.420	19.642	19.653	1.00	11.96		A	C
ANISOU	3353	CA	ASP A 554	1381	1590	1571	13	-86	3	A	C

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ATOM	3355	CB	ASP	A	554	6.573	18.668	19.869	1.00	12.72		A	C
ANISOU	3355	CB	ASP	A	554	1583	1552	1699	82	-66	97	A	C
ATOM	3358	CG	ASP	A	554	7.240	18.198	18.598	1.00	13.22		A	C
ANISOU	3358	CG	ASP	A	554	1635	1689	1700	-87	-81	88	A	C
ATOM	3359	OD1	ASP	A	554	6.637	18.167	17.485	1.00	13.26		A	O
ANISOU	3359	OD1	ASP	A	554	1556	1910	1569	117	-28	-13	A	O
ATOM	3360	OD2	ASP	A	554	8.431	17.760	18.650	1.00	15.37		A	O
ANISOU	3360	OD2	ASP	A	554	1700	2241	1898	294	30	-24	A	O
ATOM	3361	C	ASP	A	554	4.549	19.667	20.905	1.00	11.53		A	C
ANISOU	3361	C	ASP	A	554	1414	1460	1505	24	-120	52	A	C
ATOM	3362	O	ASP	A	554	3.646	18.822	21.021	1.00	11.84		A	O
ANISOU	3362	O	ASP	A	554	1407	1587	1502	-52	-17	76	A	O
ATOM	3363	N	VAL	A	555	4.832	20.572	21.857	1.00	10.94		A	N
ANISOU	3363	N	VAL	A	555	1326	1388	1441	38	-66	38	A	N
ATOM	3365	CA	VAL	A	555	3.991	20.676	23.051	1.00	11.19		A	C
ANISOU	3365	CA	VAL	A	555	1389	1444	1417	10	-56	20	A	C
ATOM	3367	CB	VAL	A	555	4.540	21.666	24.075	1.00	11.02		A	C
ANISOU	3367	CB	VAL	A	555	1368	1305	1512	-22	-26	10	A	C
ATOM	3369	CG1	VAL	A	555	3.491	22.043	25.110	1.00	12.32		A	C
ANISOU	3369	CG1	VAL	A	555	1473	1526	1681	61	-90	-30	A	C
ATOM	3373	CG2	VAL	A	555	5.811	21.118	24.728	1.00	12.43		A	C
ANISOU	3373	CG2	VAL	A	555	1469	1662	1590	-15	18	57	A	C
ATOM	3377	C	VAL	A	555	2.543	21.036	22.662	1.00	10.81		A	C
ANISOU	3377	C	VAL	A	555	1307	1344	1453	13	-25	-1	A	C
ATOM	3378	O	VAL	A	555	1.581	20.496	23.192	1.00	11.37		A	O
ANISOU	3378	O	VAL	A	555	1433	1547	1337	48	-58	27	A	O
ATOM	3379	N	TRP	A	556	2.414	21.951	21.707	1.00	10.71		A	N
ANISOU	3379	N	TRP	A	556	1164	1446	1460	63	-35	74	A	N
ATOM	3381	CA	TRP	A	556	1.100	22.355	21.191	1.00	10.86		A	C
ANISOU	3381	CA	TRP	A	556	1260	1386	1480	83	-93	30	A	C
ATOM	3383	CB	TRP	A	556	1.256	23.423	20.104	1.00	11.09		A	C
ANISOU	3383	CB	TRP	A	556	1267	1457	1488	22	-113	-59	A	C
ATOM	3386	CG	TRP	A	556	-0.066	23.871	19.576	1.00	11.43		A	C
ANISOU	3386	CG	TRP	A	556	1314	1555	1471	86	-23	96	A	C
ATOM	3387	CD1	TRP	A	556	-0.903	23.160	18.782	1.00	12.65		A	C
ANISOU	3387	CD1	TRP	A	556	1590	1619	1597	28	71	55	A	C
ATOM	3389	NE1	TRP	A	556	-2.069	23.868	18.549	1.00	12.59		A	N
ANISOU	3389	NE1	TRP	A	556	1490	1784	1507	188	19	-1	A	N
ATOM	3391	CE2	TRP	A	556	-1.963	25.089	19.169	1.00	12.53		A	C
ANISOU	3391	CE2	TRP	A	556	1603	1510	1647	-12	49	130	A	C
ATOM	3392	CD2	TRP	A	556	-0.711	25.119	19.826	1.00	10.75		A	C
ANISOU	3392	CD2	TRP	A	556	1457	1427	1198	23	40	119	A	C
ATOM	3393	CE3	TRP	A	556	-0.350	26.286	20.519	1.00	12.45		A	C
ANISOU	3393	CE3	TRP	A	556	1642	1550	1536	69	-47	-26	A	C
ATOM	3395	CZ3	TRP	A	556	-1.262	27.361	20.584	1.00	12.44		A	C
ANISOU	3395	CZ3	TRP	A	556	1530	1766	1430	31	-20	26	A	C
ATOM	3397	CH2	TRP	A	556	-2.501	27.281	19.940	1.00	12.68		A	C
ANISOU	3397	CH2	TRP	A	556	1554	1629	1635	34	41	102	A	C
ATOM	3399	CZ2	TRP	A	556	-2.868	26.173	19.222	1.00	12.83		A	C
ANISOU	3399	CZ2	TRP	A	556	1491	1733	1649	-53	164	140	A	C
ATOM	3401	C	TRP	A	556	0.370	21.113	20.660	1.00	11.24		A	C
ANISOU	3401	C	TRP	A	556	1380	1359	1532	17	19	60	A	C
ATOM	3402	O	TRP	A	556	-0.791	20.810	21.022	1.00	12.02		A	O
ANISOU	3402	O	TRP	A	556	1287	1534	1743	131	-11	47	A	O
ATOM	3403	N	SER	A	557	1.075	20.330	19.854	1.00	11.30		A	N
ANISOU	3403	N	SER	A	557	1407	1413	1471	52	-2	29	A	N
ATOM	3405	CA	SER	A	557	0.476	19.128	19.288	1.00	12.03		A	C
ANISOU	3405	CA	SER	A	557	1449	1508	1613	1	10	5	A	C
ATOM	3407	CB	SER	A	557	1.465	18.444	18.346	1.00	13.00		A	C
ANISOU	3407	CB	SER	A	557	1640	1533	1767	112	52	-13	A	C
ATOM	3410	OG	SER	A	557	2.009	19.315	17.374	1.00	15.42		A	O
ANISOU	3410	OG	SER	A	557	1776	2020	2062	-41	-59	106	A	O

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Figure 1A – 55

ATOM	3412	C	SER	A	557	0.060	18.145	20.366	1.00	11.73		A	C
ANISOU	3412	C	SER	A	557	1459	1492	1506	-12	-52	-21	A	C
ATOM	3413	O	SER	A	557	-0.974	17.496	20.256	1.00	12.51		A	O
ANISOU	3413	O	SER	A	557	1421	1684	1647	-44	-70	16	A	O
ATOM	3414	N	PHE	A	558	0.893	18.018	21.393	1.00	10.82		A	N
ANISOU	3414	N	PHE	A	558	1212	1471	1426	-41	-15	85	A	N
ATOM	3416	CA	PHE	A	558	0.595	17.184	22.517	1.00	11.22		A	C
ANISOU	3416	CA	PHE	A	558	1438	1438	1384	43	13	42	A	C
ATOM	3418	CB	PHE	A	558	1.763	17.190	23.515	1.00	11.26		A	C
ANISOU	3418	CB	PHE	A	558	1319	1542	1416	73	62	-16	A	C
ATOM	3421	CG	PHE	A	558	1.512	16.298	24.715	1.00	11.74		A	C
ANISOU	3421	CG	PHE	A	558	1236	1645	1577	44	54	108	A	C
ATOM	3422	CD1	PHE	A	558	1.547	14.929	24.575	1.00	13.45		A	C
ANISOU	3422	CD1	PHE	A	558	1897	1756	1455	2	-64	8	A	C
ATOM	3424	CE1	PHE	A	558	1.278	14.074	25.646	1.00	13.04		A	C
ANISOU	3424	CE1	PHE	A	558	1787	1511	1654	0	125	43	A	C
ATOM	3426	CZ	PHE	A	558	1.004	14.614	26.872	1.00	11.29		A	C
ANISOU	3426	CZ	PHE	A	558	1219	1676	1391	-91	36	175	A	C
ATOM	3428	CE2	PHE	A	558	0.937	15.948	27.025	1.00	13.23		A	C
ANISOU	3428	CE2	PHE	A	558	1732	1792	1503	-38	126	-15	A	C
ATOM	3430	CD2	PHE	A	558	1.206	16.819	25.950	1.00	12.06		A	C
ANISOU	3430	CD2	PHE	A	558	1584	1504	1491	-5	-100	83	A	C
ATOM	3432	C	PHE	A	558	-0.724	17.589	23.188	1.00	11.02		A	C
ANISOU	3432	C	PHE	A	558	1389	1408	1387	11	-1	97	A	C
ATOM	3433	O	PHE	A	558	-1.510	16.729	23.636	1.00	12.18		A	O
ANISOU	3433	O	PHE	A	558	1476	1693	1459	-46	120	51	A	O
ATOM	3434	N	GLY	A	559	-0.971	18.893	23.271	1.00	11.81		A	N
ANISOU	3434	N	GLY	A	559	1428	1546	1513	45	-14	-18	A	N
ATOM	3436	CA	GLY	A	559	-2.237	19.354	23.765	1.00	11.71		A	C
ANISOU	3436	CA	GLY	A	559	1466	1488	1495	30	59	3	A	C
ATOM	3439	C	GLY	A	559	-3.397	18.858	22.949	1.00	12.35		A	C
ANISOU	3439	C	GLY	A	559	1508	1562	1620	61	52	50	A	C
ATOM	3440	O	GLY	A	559	-4.442	18.440	23.515	1.00	12.78		A	O
ANISOU	3440	O	GLY	A	559	1420	1684	1749	51	131	75	A	O
ATOM	3441	N	VAL	A	560	-3.252	18.912	21.624	1.00	11.65		A	N
ANISOU	3441	N	VAL	A	560	1380	1522	1523	100	40	-42	A	N
ATOM	3443	CA	VAL	A	560	-4.303	18.418	20.739	1.00	12.04		A	C
ANISOU	3443	CA	VAL	A	560	1442	1571	1561	40	25	-22	A	C
ATOM	3445	CB	VAL	A	560	-4.006	18.722	19.278	1.00	12.28		A	C
ANISOU	3445	CB	VAL	A	560	1397	1559	1708	37	-35	35	A	C
ATOM	3447	CG1	VAL	A	560	-5.091	18.141	18.368	1.00	13.01		A	C
ANISOU	3447	CG1	VAL	A	560	1559	1812	1569	106	-61	-62	A	C
ATOM	3451	CG2	VAL	A	560	-3.871	20.219	19.065	1.00	12.23		A	C
ANISOU	3451	CG2	VAL	A	560	1572	1545	1531	50	34	-21	A	C
ATOM	3455	C	VAL	A	560	-4.474	16.899	20.954	1.00	12.46		A	C
ANISOU	3455	C	VAL	A	560	1489	1608	1636	13	-53	-3	A	C
ATOM	3456	O	VAL	A	560	-5.610	16.391	21.053	1.00	12.87		A	O
ANISOU	3456	O	VAL	A	560	1396	1822	1670	-37	-172	118	A	O
ATOM	3457	N	LEU	A	561	-3.351	16.187	21.080	1.00	12.38		A	N
ANISOU	3457	N	LEU	A	561	1468	1542	1691	1	-21	7	A	N
ATOM	3459	CA	LEU	A	561	-3.355	14.743	21.312	1.00	12.51		A	C
ANISOU	3459	CA	LEU	A	561	1477	1592	1684	84	-50	-12	A	C
ATOM	3461	CB	LEU	A	561	-1.892	14.260	21.382	1.00	12.26		A	C
ANISOU	3461	CB	LEU	A	561	1362	1678	1615	40	7	44	A	C
ATOM	3464	CG	LEU	A	561	-1.692	12.769	21.521	1.00	14.33		A	C
ANISOU	3464	CG	LEU	A	561	1597	1911	1934	95	-16	-22	A	C
ATOM	3466	CD1	LEU	A	561	-0.284	12.456	21.017	1.00	15.93		A	C
ANISOU	3466	CD1	LEU	A	561	1786	2072	2193	89	-3	58	A	C
ATOM	3470	CD2	LEU	A	561	-1.823	12.362	22.904	1.00	15.92		A	C
ANISOU	3470	CD2	LEU	A	561	1843	2097	2107	112	72	44	A	C
ATOM	3474	C	LEU	A	561	-4.129	14.415	22.605	1.00	12.95		A	C
ANISOU	3474	C	LEU	A	561	1633	1541	1744	21	-57	79	A	C

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Figure 1A – 56

ATOM	3475	O	LEU A 561	-4.943	13.489	22.648	1.00	13.21		A	O
ANISOU	3475	O	LEU A 561	1552	1740	1727	-100	-60	35	A	O
ATOM	3476	N	MET A 562	-3.913	15.202	23.657	1.00	12.96		A	N
ANISOU	3476	N	MET A 562	1591	1640	1691	-22	-26	49	A	N
ATOM	3478	CA	MET A 562	-4.628	14.974	24.907	1.00	13.47		A	C
ANISOU	3478	CA	MET A 562	1592	1748	1778	27	26	59	A	C
ATOM	3480	CB	MET A 562	-4.151	15.900	26.007	1.00	14.05		A	C
ANISOU	3480	CB	MET A 562	1695	1871	1769	-8	84	34	A	C
ATOM	3483	CG	AMET A 562	-2.776	15.707	26.595	0.50	15.35		A	C
ANISOU	3483	CG	AMET A 562	1836	2088	1908	-15	3	13	A	C
ATOM	3484	CG	BMET A 562	-2.839	15.359	26.549	0.50	14.88		A	C
ANISOU	3484	CG	BMET A 562	1750	2088	1814	-33	45	26	A	C
ATOM	3489	SD	AMET A 562	-2.394	17.016	27.833	0.50	16.12		A	S
ANISOU	3489	SD	AMET A 562	1989	2037	2098	22	-16	-26	A	S
ATOM	3490	SD	BMET A 562	-2.280	16.064	28.076	0.50	14.40		A	S
ANISOU	3490	SD	BMET A 562	1776	2007	1686	66	-47	244	A	S
ATOM	3491	CE	AMET A 562	-3.588	16.540	29.084	0.50	17.03		A	C
ANISOU	3491	CE	AMET A 562	2092	2190	2187	4	63	51	A	C
ATOM	3492	CE	BMET A 562	-2.209	17.774	27.600	0.50	12.81		A	C
ANISOU	3492	CE	BMET A 562	1650	1667	1548	7	-63	-12	A	C
ATOM	3499	C	MET A 562	-6.129	15.180	24.678	1.00	13.50		A	C
ANISOU	3499	C	MET A 562	1548	1769	1809	-33	-19	67	A	C
ATOM	3500	O	MET A 562	-6.957	14.417	25.178	1.00	14.38		A	O
ANISOU	3500	O	MET A 562	1641	1901	1922	-35	117	200	A	O
ATOM	3501	N	TRP A 563	-6.484	16.256	23.988	1.00	13.09		A	N
ANISOU	3501	N	TRP A 563	1510	1709	1751	-58	-1	50	A	N
ATOM	3503	CA	TRP A 563	-7.887	16.483	23.677	1.00	13.51		A	C
ANISOU	3503	CA	TRP A 563	1639	1718	1775	-4	-28	0	A	C
ATOM	3505	CB	TRP A 563	-8.032	17.758	22.820	1.00	14.22		A	C
ANISOU	3505	CB	TRP A 563	1784	1743	1875	-55	-9	44	A	C
ATOM	3508	CG	TRP A 563	-9.474	18.091	22.567	1.00	14.32		A	C
ANISOU	3508	CG	TRP A 563	1779	1840	1822	-82	-67	103	A	C
ATOM	3509	CD1	TRP A 563	-10.261	18.944	23.274	1.00	16.27		A	C
ANISOU	3509	CD1	TRP A 563	1923	2159	2100	-61	21	144	A	C
ATOM	3511	NE1	TRP A 563	-11.542	18.942	22.762	1.00	16.59		A	N
ANISOU	3511	NE1	TRP A 563	1978	2135	2190	-60	34	272	A	N
ATOM	3513	CE2	TRP A 563	-11.584	18.096	21.687	1.00	16.91		A	C
ANISOU	3513	CE2	TRP A 563	2038	2282	2104	-49	-136	94	A	C
ATOM	3514	CD2	TRP A 563	-10.301	17.530	21.542	1.00	14.89		A	C
ANISOU	3514	CD2	TRP A 563	1870	1952	1833	-122	-59	190	A	C
ATOM	3515	CE3	TRP A 563	-10.082	16.612	20.514	1.00	14.64		A	C
ANISOU	3515	CE3	TRP A 563	1621	1892	2047	-2	-15	198	A	C
ATOM	3517	CZ3	TRP A 563	-11.142	16.295	19.673	1.00	17.46		A	C
ANISOU	3517	CZ3	TRP A 563	2292	2114	2228	-118	-150	42	A	C
ATOM	3519	CH2	TRP A 563	-12.402	16.876	19.865	1.00	17.86		A	C
ANISOU	3519	CH2	TRP A 563	2139	2322	2323	-153	-45	135	A	C
ATOM	3521	CZ2	TRP A 563	-12.645	17.755	20.849	1.00	17.27		A	C
ANISOU	3521	CZ2	TRP A 563	1839	2319	2402	-144	30	168	A	C
ATOM	3523	C	TRP A 563	-8.485	15.243	22.982	1.00	14.35		A	C
ANISOU	3523	C	TRP A 563	1704	1811	1935	-53	31	35	A	C
ATOM	3524	O	TRP A 563	-9.587	14.780	23.342	1.00	14.99		A	O
ANISOU	3524	O	TRP A 563	1723	1800	2172	-52	33	90	A	O
ATOM	3525	N	GLU A 564	-7.781	14.725	21.973	1.00	13.50		A	N
ANISOU	3525	N	GLU A 564	1539	1779	1810	-10	-14	49	A	N
ATOM	3527	CA	GLU A 564	-8.214	13.522	21.262	1.00	14.54		A	C
ANISOU	3527	CA	GLU A 564	1732	1859	1932	8	-57	63	A	C
ATOM	3529	CB	GLU A 564	-7.185	13.101	20.239	1.00	14.74		A	C
ANISOU	3529	CB	GLU A 564	1825	1836	1938	1	-71	57	A	C
ATOM	3532	CG	GLU A 564	-6.972	14.005	19.041	1.00	14.77		A	C
ANISOU	3532	CG	GLU A 564	1719	1924	1968	-141	-54	25	A	C
ATOM	3535	CD	GLU A 564	-5.968	13.427	18.088	1.00	14.80		A	C
ANISOU	3535	CD	GLU A 564	1751	1921	1951	4	-142	98	A	C



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ATOM	3536	OE1	GLU	A	564	-4.746	13.660	18.281	1.00	14.33		A	O
ANISOU	3536	OE1	GLU	A	564	1570	1906	1966	-287	-124	-56	A	O
ATOM	3537	OE2	GLU	A	564	-6.359	12.670	17.166	1.00	17.01		A	O
ANISOU	3537	OE2	GLU	A	564	1916	2264	2281	-37	-88	-247	A	O
ATOM	3538	C	GLU	A	564	-8.445	12.351	22.223	1.00	14.84		A	C
ANISOU	3538	C	GLU	A	564	1737	1861	2041	-73	17	36	A	C
ATOM	3539	O	GLU	A	564	-9.456	11.633	22.145	1.00	16.55		A	O
ANISOU	3539	O	GLU	A	564	1706	1986	2593	-116	71	14	A	O
ATOM	3540	N	ALA	A	565	-7.496	12.165	23.131	1.00	14.45		A	N
ANISOU	3540	N	ALA	A	565	1713	1813	1961	-16	32	110	A	N
ATOM	3542	CA	ALA	A	565	-7.520	11.041	24.074	1.00	15.69		A	C
ANISOU	3542	CA	ALA	A	565	1975	1959	2025	-25	47	74	A	C
ATOM	3544	CB	ALA	A	565	-6.216	10.985	24.842	1.00	15.91		A	C
ANISOU	3544	CB	ALA	A	565	1972	1998	2073	-14	27	156	A	C
ATOM	3548	C	ALA	A	565	-8.684	11.117	25.033	1.00	16.34		A	C
ANISOU	3548	C	ALA	A	565	2040	2077	2089	-39	20	117	A	C
ATOM	3549	O	ALA	A	565	-9.217	10.083	25.418	1.00	18.09		A	O
ANISOU	3549	O	ALA	A	565	2309	2129	2434	-137	100	135	A	O
ATOM	3550	N	PHE	A	566	-9.094	12.317	25.401	1.00	16.88		A	N
ANISOU	3550	N	PHE	A	566	2099	2132	2182	1	93	122	A	N
ATOM	3552	CA	PHE	A	566	-10.213	12.468	26.335	1.00	18.50		A	C
ANISOU	3552	CA	PHE	A	566	2300	2338	2390	31	88	122	A	C
ATOM	3554	CB	PHE	A	566	-9.952	13.579	27.330	1.00	18.91		A	C
ANISOU	3554	CB	PHE	A	566	2332	2481	2372	52	104	130	A	C
ATOM	3557	CG	PHE	A	566	-8.971	13.204	28.377	1.00	20.42		A	C
ANISOU	3557	CG	PHE	A	566	2644	2655	2459	70	61	30	A	C
ATOM	3558	CD1	PHE	A	566	-9.357	12.467	29.457	1.00	21.30		A	C
ANISOU	3558	CD1	PHE	A	566	2791	2584	2716	38	25	147	A	C
ATOM	3560	CE1	PHE	A	566	-8.424	12.106	30.422	1.00	22.13		A	C
ANISOU	3560	CE1	PHE	A	566	2959	2738	2709	65	-35	-16	A	C
ATOM	3562	CZ	PHE	A	566	-7.119	12.452	30.270	1.00	23.52		A	C
ANISOU	3562	CZ	PHE	A	566	3041	2973	2921	79	-37	23	A	C
ATOM	3564	CE2	PHE	A	566	-6.722	13.176	29.165	1.00	23.40		A	C
ANISOU	3564	CE2	PHE	A	566	2998	2948	2942	96	-125	28	A	C
ATOM	3566	CD2	PHE	A	566	-7.661	13.546	28.237	1.00	20.38		A	C
ANISOU	3566	CD2	PHE	A	566	2595	2557	2592	22	-47	40	A	C
ATOM	3568	C	PHE	A	566	-11.546	12.643	25.611	1.00	18.97		A	C
ANISOU	3568	C	PHE	A	566	2277	2452	2476	59	68	74	A	C
ATOM	3569	O	PHE	A	566	-12.599	12.816	26.259	1.00	20.63		A	O
ANISOU	3569	O	PHE	A	566	2338	2780	2718	-65	241	241	A	O
ATOM	3570	N	SER	A	567	-11.508	12.588	24.283	1.00	19.29		A	N
ANISOU	3570	N	SER	A	567	2243	2514	2570	15	75	42	A	N
ATOM	3572	CA	SER	A	567	-12.699	12.712	23.443	1.00	20.18		A	C
ANISOU	3572	CA	SER	A	567	2417	2658	2592	8	58	76	A	C
ATOM	3574	CB	SER	A	567	-12.501	13.851	22.442	1.00	19.82		A	C
ANISOU	3574	CB	SER	A	567	2317	2603	2610	11	1	93	A	C
ATOM	3577	OG	SER	A	567	-12.368	15.074	23.112	1.00	19.43		A	O
ANISOU	3577	OG	SER	A	567	2162	2694	2524	-27	114	167	A	O
ATOM	3579	C	SER	A	567	-12.981	11.419	22.693	1.00	20.81		A	C
ANISOU	3579	C	SER	A	567	2495	2666	2746	-31	56	54	A	C
ATOM	3580	O	SER	A	567	-13.478	11.434	21.569	1.00	22.17		A	O
ANISOU	3580	O	SER	A	567	2670	2728	3026	-125	82	40	A	O
ATOM	3581	N	TYR	A	568	-12.645	10.282	23.280	1.00	22.92		A	N
ANISOU	3581	N	TYR	A	568	2792	2927	2990	-33	22	79	A	N
ATOM	3583	CA	TYR	A	568	-12.891	9.000	22.615	1.00	24.11		A	C
ANISOU	3583	CA	TYR	A	568	2963	3058	3140	-30	-56	5	A	C
ATOM	3585	CB	TYR	A	568	-14.405	8.767	22.396	1.00	25.00		A	C
ANISOU	3585	CB	TYR	A	568	3039	3134	3325	-34	-73	4	A	C
ATOM	3588	CG	TYR	A	568	-15.177	8.655	23.661	1.00	28.14		A	C
ANISOU	3588	CG	TYR	A	568	3470	3669	3553	-46	2	14	A	C
ATOM	3589	CD1	TYR	A	568	-15.054	7.542	24.465	1.00	31.22		A	C
ANISOU	3589	CD1	TYR	A	568	3970	3926	3966	34	-18	91	A	C

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ATOM	3591	CE1	TYR	A	568	-15.746	7.437	25.647	1.00	32.61		A	C
ANISOU	3591	CE1	TYR	A	568	4023	4227	4137	37	49	47	A	C
ATOM	3593	CZ	TYR	A	568	-16.583	8.445	26.041	1.00	33.77		A	C
ANISOU	3593	CZ	TYR	A	568	4265	4267	4298	63	54	47	A	C
ATOM	3594	OH	TYR	A	568	-17.282	8.313	27.225	1.00	34.57		A	O
ANISOU	3594	OH	TYR	A	568	4527	4407	4201	90	27	179	A	O
ATOM	3596	CE2	TYR	A	568	-16.739	9.569	25.256	1.00	32.89		A	C
ANISOU	3596	CE2	TYR	A	568	4014	4272	4208	4	88	79	A	C
ATOM	3598	CD2	TYR	A	568	-16.035	9.670	24.070	1.00	31.32		A	C
ANISOU	3598	CD2	TYR	A	568	3993	3939	3967	107	-3	-19	A	C
ATOM	3600	C	TYR	A	568	-12.217	8.896	21.268	1.00	24.04		A	C
ANISOU	3600	C	TYR	A	568	2964	3016	3155	-79	-47	15	A	C
ATOM	3601	O	TYR	A	568	-12.759	8.291	20.351	1.00	24.98		A	O
ANISOU	3601	O	TYR	A	568	3085	3061	3345	-201	-80	28	A	O
ATOM	3602	N	GLY	A	569	-11.052	9.520	21.100	1.00	22.51		A	N
ANISOU	3602	N	GLY	A	569	2753	2791	3008	-99	-59	4	A	N
ATOM	3604	CA	GLY	A	569	-10.356	9.428	19.846	1.00	23.11		A	C
ANISOU	3604	CA	GLY	A	569	2863	2875	3041	-92	-62	-3	A	C
ATOM	3607	C	GLY	A	569	-10.939	10.228	18.709	1.00	23.56		A	C
ANISOU	3607	C	GLY	A	569	2944	2955	3050	-103	-41	0	A	C
ATOM	3608	O	GLY	A	569	-10.496	10.062	17.576	1.00	24.91		A	O
ANISOU	3608	O	GLY	A	569	3029	3229	3207	-107	-118	17	A	O
ATOM	3609	N	GLN	A	570	-11.855	11.143	19.002	1.00	24.02		A	N
ANISOU	3609	N	GLN	A	570	2892	3097	3135	-133	-17	99	A	N
ATOM	3611	CA	GLN	A	570	-12.438	11.984	17.962	1.00	24.74		A	C
ANISOU	3611	CA	GLN	A	570	3070	3152	3176	-101	-15	60	A	C
ATOM	3613	CB	GLN	A	570	-13.596	12.764	18.523	1.00	25.89		A	C
ANISOU	3613	CB	GLN	A	570	3167	3347	3322	-15	-2	87	A	C
ATOM	3616	CG	GLN	A	570	-14.849	11.903	18.675	0.70	28.84		A	C
ANISOU	3616	CG	GLN	A	570	3610	3631	3714	-122	2	50	A	C
ATOM	3619	CD	GLN	A	570	-16.037	12.511	17.972	0.70	31.90		A	C
ANISOU	3619	CD	GLN	A	570	3933	4084	4103	105	-47	4	A	C
ATOM	3620	OE1	GLN	A	570	-15.882	13.164	16.935	0.70	34.10		A	O
ANISOU	3620	OE1	GLN	A	570	4403	4265	4288	11	85	8	A	O
ATOM	3621	NE2	GLN	A	570	-17.224	12.314	18.532	0.70	33.68		A	N
ANISOU	3621	NE2	GLN	A	570	4218	4288	4287	-68	57	70	A	N
ATOM	3624	C	GLN	A	570	-11.430	12.952	17.355	1.00	23.28		A	C
ANISOU	3624	C	GLN	A	570	2898	2993	2953	-71	-23	78	A	C
ATOM	3625	O	GLN	A	570	-10.458	13.319	17.983	1.00	21.69		A	O
ANISOU	3625	O	GLN	A	570	2630	2841	2768	-15	7	85	A	O
ATOM	3626	N	LYS	A	571	-11.683	13.333	16.113	1.00	23.03		A	N
ANISOU	3626	N	LYS	A	571	2851	2946	2950	-126	-18	65	A	N
ATOM	3628	CA	LYS	A	571	-10.815	14.233	15.358	1.00	22.26		A	C
ANISOU	3628	CA	LYS	A	571	2752	2809	2896	-31	6	32	A	C
ATOM	3630	CB	LYS	A	571	-11.213	14.235	13.893	1.00	23.77		A	C
ANISOU	3630	CB	LYS	A	571	3006	3025	2998	-72	20	16	A	C
ATOM	3633	CG	ALYS	A	571	-11.056	12.890	13.191	0.70	27.15		A	C
ANISOU	3633	CG	ALYS	A	571	3508	3352	3454	68	-24	-54	A	C
ATOM	3634	CG	BLYS	A	571	-11.100	12.959	13.024	0.30	24.78		A	C
ANISOU	3634	CG	BLYS	A	571	3151	3110	3155	6	4	-15	A	C
ATOM	3639	CD	ALYS	A	571	-11.832	11.736	13.836	0.70	30.40		A	C
ANISOU	3639	CD	ALYS	A	571	3840	3857	3852	-40	20	14	A	C
ATOM	3640	CD	BLYS	A	571	-10.838	11.629	13.712	0.30	25.53		A	C
ANISOU	3640	CD	BLYS	A	571	3238	3230	3231	10	-1	27	A	C
ATOM	3645	CE	ALYS	A	571	-13.344	11.883	13.739	0.70	31.62		A	C
ANISOU	3645	CE	ALYS	A	571	3913	4025	4073	-25	-60	-13	A	C
ATOM	3646	CE	BLYS	A	571	-11.751	10.548	13.125	0.30	26.22		A	C
ANISOU	3646	CE	BLYS	A	571	3340	3297	3325	-14	-11	-22	A	C
ATOM	3651	NZ	ALYS	A	571	-13.997	11.008	14.740	0.70	33.96		A	N
ANISOU	3651	NZ	ALYS	A	571	4295	4457	4151	-47	7	73	A	N
ATOM	3652	NZ	BLYS	A	571	-11.226	9.181	13.323	0.30	26.59		A	N
ANISOU	3652	NZ	BLYS	A	571	3431	3331	3338	30	-5	0	A	N

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ATOM	3659	C	LYS A 571	-11.016	15.643	15.903	1.00	20.15		A	C
ANISOU	3659	C	LYS A 571	2384	2641	2629	-64	7	23	A	C
ATOM	3660	O	LYS A 571	-12.129	16.047	16.245	1.00	20.06		A	O
ANISOU	3660	O	LYS A 571	2325	2661	2636	-135	-20	-31	A	O
ATOM	3661	N	PRO A 572	-9.949	16.421	15.989	1.00	17.50		A	N
ANISOU	3661	N	PRO A 572	2060	2301	2287	13	-25	54	A	N
ATOM	3662	CA	PRO A 572	-10.049	17.767	16.522	1.00	15.97		A	C
ANISOU	3662	CA	PRO A 572	1852	2157	2057	-15	46	34	A	C
ATOM	3664	CB	PRO A 572	-8.603	18.119	16.858	1.00	16.62		A	C
ANISOU	3664	CB	PRO A 572	2004	2129	2180	6	-57	29	A	C
ATOM	3667	CG	PRO A 572	-7.819	17.318	15.890	1.00	17.31		A	C
ANISOU	3667	CG	PRO A 572	1994	2372	2208	-44	15	-89	A	C
ATOM	3670	CD	PRO A 572	-8.564	16.037	15.659	1.00	17.57		A	C
ANISOU	3670	CD	PRO A 572	2106	2253	2314	72	32	-10	A	C
ATOM	3673	C	PRO A 572	-10.629	18.746	15.491	1.00	14.76		A	C
ANISOU	3673	C	PRO A 572	1706	1967	1932	-15	30	-2	A	C
ATOM	3674	O	PRO A 572	-10.565	18.490	14.290	1.00	15.65		A	O
ANISOU	3674	O	PRO A 572	1717	2142	2084	20	-6	-97	A	O
ATOM	3675	N	TYR A 573	-11.217	19.833	15.988	1.00	14.82		A	N
ANISOU	3675	N	TYR A 573	1679	1996	1954	14	65	-38	A	N
ATOM	3677	CA	TYR A 573	-11.762	20.911	15.172	1.00	14.60		A	C
ANISOU	3677	CA	TYR A 573	1734	1911	1900	-29	44	-1	A	C
ATOM	3679	CB	TYR A 573	-10.627	21.708	14.516	1.00	14.02		A	C
ANISOU	3679	CB	TYR A 573	1570	1835	1919	-22	-16	14	A	C
ATOM	3682	CG	TYR A 573	-9.606	22.265	15.487	1.00	12.65		A	C
ANISOU	3682	CG	TYR A 573	1587	1729	1487	21	1	93	A	C
ATOM	3683	CD1	TYR A 573	-9.836	23.376	16.243	1.00	11.56		A	C
ANISOU	3683	CD1	TYR A 573	970	1731	1691	62	128	125	A	C
ATOM	3685	CE1	TYR A 573	-8.900	23.859	17.128	1.00	13.27		A	C
ANISOU	3685	CE1	TYR A 573	1657	1706	1679	187	31	-6	A	C
ATOM	3687	CZ	TYR A 573	-7.688	23.209	17.271	1.00	12.42		A	C
ANISOU	3687	CZ	TYR A 573	1477	1664	1576	-5	8	225	A	C
ATOM	3688	OH	TYR A 573	-6.718	23.676	18.146	1.00	14.04		A	O
ANISOU	3688	OH	TYR A 573	1483	1939	1910	-48	5	34	A	O
ATOM	3690	CE2	TYR A 573	-7.448	22.101	16.523	1.00	13.59		A	C
ANISOU	3690	CE2	TYR A 573	1701	1930	1532	25	6	67	A	C
ATOM	3692	CD2	TYR A 573	-8.384	21.637	15.639	1.00	13.60		A	C
ANISOU	3692	CD2	TYR A 573	1435	2040	1691	79	189	0	A	C
ATOM	3694	C	TYR A 573	-12.698	20.372	14.103	1.00	15.57		A	C
ANISOU	3694	C	TYR A 573	1808	2078	2028	13	41	35	A	C
ATOM	3695	O	TYR A 573	-12.639	20.734	12.927	1.00	16.47		A	O
ANISOU	3695	O	TYR A 573	1600	2506	2150	-3	-101	8	A	O
ATOM	3696	N	ARG A 574	-13.581	19.486	14.524	1.00	17.44		A	N
ANISOU	3696	N	ARG A 574	2019	2284	2322	-87	-44	7	A	N
ATOM	3698	CA	ARG A 574	-14.436	18.876	13.539	1.00	18.10		A	C
ANISOU	3698	CA	ARG A 574	2146	2384	2346	-49	-26	17	A	C
ATOM	3700	CB	ARG A 574	-15.223	17.731	14.111	1.00	20.58		A	C
ANISOU	3700	CB	ARG A 574	2514	2601	2702	-14	11	89	A	C
ATOM	3703	CG	ARG A 574	-16.466	18.055	14.748	1.00	20.61		A	C
ANISOU	3703	CG	ARG A 574	2519	2560	2750	105	132	122	A	C
ATOM	3706	CD	ARG A 574	-17.380	16.825	15.030	1.00	20.65		A	C
ANISOU	3706	CD	ARG A 574	2608	2591	2647	-2	-41	22	A	C
ATOM	3709	NE	ARG A 574	-18.358	17.218	16.041	1.00	19.72		A	N
ANISOU	3709	NE	ARG A 574	2370	2430	2690	103	-23	59	A	N
ATOM	3711	CZ	ARG A 574	-18.826	16.446	17.029	1.00	20.23		A	C
ANISOU	3711	CZ	ARG A 574	2432	2578	2674	-63	-18	-11	A	C
ATOM	3712	NH1	ARG A 574	-18.439	15.196	17.173	1.00	22.68		A	N
ANISOU	3712	NH1	ARG A 574	2697	2741	3177	122	70	-19	A	N
ATOM	3715	NH2	ARG A 574	-19.690	16.936	17.894	1.00	19.36		A	N
ANISOU	3715	NH2	ARG A 574	2282	2510	2564	44	-45	58	A	N
ATOM	3718	C	ARG A 574	-15.296	19.904	12.825	1.00	16.79		A	C
ANISOU	3718	C	ARG A 574	1871	2270	2235	-81	-39	4	A	C

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ATOM	3719	O	ARG A 574	-15.732	20.941	13.375	1.00	16.06		A	O
ANISOU	3719	O	ARG A 574	1606	2282	2211	-176	-186	75	A	O
ATOM	3720	N	GLY A 575	-15.457	19.632	11.542	1.00	17.48		A	N
ANISOU	3720	N	GLY A 575	1954	2394	2292	-71	-17	-14	A	N
ATOM	3722	CA	GLY A 575	-16.235	20.479	10.664	1.00	17.35		A	C
ANISOU	3722	CA	GLY A 575	2072	2334	2187	-41	-64	7	A	C
ATOM	3725	C	GLY A 575	-15.539	21.722	10.156	1.00	18.70		A	C
ANISOU	3725	C	GLY A 575	2284	2478	2344	-42	-76	78	A	C
ATOM	3726	O	GLY A 575	-16.124	22.510	9.404	1.00	20.27		A	O
ANISOU	3726	O	GLY A 575	2261	2960	2478	-66	-254	205	A	O
ATOM	3727	N	MET A 576	-14.307	21.937	10.622	1.00	17.81		A	N
ANISOU	3727	N	MET A 576	2046	2463	2258	-18	-28	59	A	N
ATOM	3729	CA	MET A 576	-13.572	23.143	10.299	1.00	18.41		A	C
ANISOU	3729	CA	MET A 576	2239	2407	2346	36	-8	-7	A	C
ATOM	3731	CB	MET A 576	-12.987	23.760	11.564	1.00	17.66		A	C
ANISOU	3731	CB	MET A 576	2177	2375	2154	10	-14	106	A	C
ATOM	3734	CG	MET A 576	-13.983	24.058	12.633	1.00	17.90		A	C
ANISOU	3734	CG	MET A 576	2086	2412	2301	36	-62	13	A	C
ATOM	3737	SD	MET A 576	-13.270	24.772	14.104	1.00	17.17		A	S
ANISOU	3737	SD	MET A 576	1812	2672	2038	32	-93	168	A	S
ATOM	3738	CE	MET A 576	-12.715	26.292	13.475	1.00	17.28		A	C
ANISOU	3738	CE	MET A 576	1879	2579	2106	-41	78	75	A	C
ATOM	3742	C	MET A 576	-12.432	22.878	9.308	1.00	18.79		A	C
ANISOU	3742	C	MET A 576	2244	2533	2360	-16	-24	-26	A	C
ATOM	3743	O	MET A 576	-11.803	21.835	9.356	1.00	19.04		A	O
ANISOU	3743	O	MET A 576	2224	2622	2387	-26	24	12	A	O
ATOM	3744	N	LYS A 577	-12.231	23.817	8.408	1.00	20.32		A	N
ANISOU	3744	N	LYS A 577	2419	2702	2598	-43	-27	-9	A	N
ATOM	3746	CA	LYS A 577	-11.114	23.797	7.487	1.00	21.50		A	C
ANISOU	3746	CA	LYS A 577	2623	2849	2694	-56	9	-5	A	C
ATOM	3748	CB	LYS A 577	-11.351	24.781	6.353	1.00	22.76		A	C
ANISOU	3748	CB	LYS A 577	2749	3045	2851	-44	26	43	A	C
ATOM	3751	CG	LYS A 577	-12.550	24.443	5.453	1.00	26.27		A	C
ANISOU	3751	CG	LYS A 577	3192	3445	3344	-74	-100	-47	A	C
ATOM	3754	CD	LYS A 577	-12.683	25.389	4.260	1.00	30.72		A	C
ANISOU	3754	CD	LYS A 577	3891	3994	3787	3	-7	102	A	C
ATOM	3757	CE	LYS A 577	-12.437	26.858	4.600	1.00	34.13		A	C
ANISOU	3757	CE	LYS A 577	4321	4293	4351	-15	-27	-33	A	C
ATOM	3760	NZ	LYS A 577	-12.730	27.799	3.448	1.00	37.32		A	N
ANISOU	3760	NZ	LYS A 577	4843	4674	4661	6	-43	118	A	N
ATOM	3764	C	LYS A 577	-9.880	24.255	8.259	1.00	20.91		A	C
ANISOU	3764	C	LYS A 577	2586	2767	2591	-44	9	44	A	C
ATOM	3765	O	LYS A 577	-9.980	25.031	9.199	1.00	18.87		A	O
ANISOU	3765	O	LYS A 577	2332	2517	2318	-44	19	115	A	O
ATOM	3766	N	GLY A 578	-8.709	23.828	7.821	1.00	21.61		A	N
ANISOU	3766	N	GLY A 578	2687	2883	2641	-23	30	10	A	N
ATOM	3768	CA	GLY A 578	-7.482	24.303	8.447	1.00	21.72		A	C
ANISOU	3768	CA	GLY A 578	2634	2952	2664	-1	64	14	A	C
ATOM	3771	C	GLY A 578	-7.383	25.807	8.596	1.00	21.87		A	C
ANISOU	3771	C	GLY A 578	2630	2998	2680	-42	68	25	A	C
ATOM	3772	O	GLY A 578	-6.974	26.304	9.641	1.00	20.73		A	O
ANISOU	3772	O	GLY A 578	2342	3027	2504	-147	226	-51	A	O
ATOM	3773	N	SER A 579	-7.755	26.546	7.556	1.00	22.18		A	N
ANISOU	3773	N	SER A 579	2738	3011	2675	-20	43	63	A	N
ATOM	3775	CA	SER A 579	-7.712	27.992	7.585	1.00	23.06		A	C
ANISOU	3775	CA	SER A 579	2916	3071	2771	-36	-12	79	A	C
ATOM	3777	CB	SER A 579	-8.050	28.550	6.191	1.00	23.97		A	C
ANISOU	3777	CB	SER A 579	3051	3153	2902	3	1	125	A	C
ATOM	3780	OG	SER A 579	-9.351	28.174	5.821	1.00	26.31		A	O
ANISOU	3780	OG	SER A 579	3449	3439	3105	-142	-165	132	A	O
ATOM	3782	C	SER A 579	-8.648	28.576	8.645	1.00	21.95		A	C
ANISOU	3782	C	SER A 579	2778	2844	2717	1	-16	115	A	C

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ATOM	3783	O	SER	A	579	-8.357	29.592	9.270	1.00	21.86		A	O
ANISOU	3783	O	SER	A	579	2747	3062	2495	-130	-11	192	A	O
ATOM	3784	N	GLU	A	580	-9.778	27.918	8.859	1.00	20.86		A	N
ANISOU	3784	N	GLU	A	580	2610	2807	2506	8	-72	90	A	N
ATOM	3786	CA	GLU	A	580	-10.723	28.372	9.874	1.00	20.51		A	C
ANISOU	3786	CA	GLU	A	580	2632	2658	2502	45	-47	86	A	C
ATOM	3788	CB	GLU	A	580	-12.044	27.652	9.704	1.00	20.70		A	C
ANISOU	3788	CB	GLU	A	580	2585	2707	2571	63	-55	83	A	C
ATOM	3791	CG	GLU	A	580	-12.831	28.124	8.479	1.00	22.23		A	C
ANISOU	3791	CG	GLU	A	580	2852	2918	2675	99	-98	107	A	C
ATOM	3794	CD	GLU	A	580	-14.023	27.254	8.159	1.00	25.10		A	C
ANISOU	3794	CD	GLU	A	580	3169	3179	3190	-64	4	26	A	C
ATOM	3795	OE1	GLU	A	580	-13.952	26.034	8.309	1.00	24.62		A	O
ANISOU	3795	OE1	GLU	A	580	3004	3283	3065	27	-143	174	A	O
ATOM	3796	OE2	GLU	A	580	-15.056	27.798	7.724	1.00	31.63		A	O
ANISOU	3796	OE2	GLU	A	580	3799	4063	4156	102	-187	212	A	O
ATOM	3797	C	GLU	A	580	-10.137	28.152	11.285	1.00	19.13		A	C
ANISOU	3797	C	GLU	A	580	2347	2533	2388	24	-80	49	A	C
ATOM	3798	O	GLU	A	580	-10.361	28.943	12.206	1.00	19.20		A	O
ANISOU	3798	O	GLU	A	580	2326	2652	2318	114	-66	127	A	O
ATOM	3799	N	VAL	A	581	-9.382	27.072	11.429	1.00	18.32		A	N
ANISOU	3799	N	VAL	A	581	2275	2454	2229	-1	-30	48	A	N
ATOM	3801	CA	VAL	A	581	-8.714	26.774	12.696	1.00	17.23		A	C
ANISOU	3801	CA	VAL	A	581	2106	2321	2118	10	8	73	A	C
ATOM	3803	CB	VAL	A	581	-8.078	25.354	12.667	1.00	16.42		A	C
ANISOU	3803	CB	VAL	A	581	2047	2270	1921	-25	4	48	A	C
ATOM	3805	CG1	VAL	A	581	-7.223	25.090	13.897	1.00	15.80		A	C
ANISOU	3805	CG1	VAL	A	581	1654	2284	2063	66	48	68	A	C
ATOM	3809	CG2	VAL	A	581	-9.150	24.301	12.530	1.00	17.27		A	C
ANISOU	3809	CG2	VAL	A	581	2166	2280	2115	12	-32	51	A	C
ATOM	3813	C	VAL	A	581	-7.689	27.874	12.997	1.00	17.04		A	C
ANISOU	3813	C	VAL	A	581	2001	2297	2175	69	26	17	A	C
ATOM	3814	O	VAL	A	581	-7.607	28.362	14.102	1.00	16.61		A	O
ANISOU	3814	O	VAL	A	581	1810	2369	2129	119	92	65	A	O
ATOM	3815	N	THR	A	582	-6.878	28.255	12.006	1.00	17.95		A	N
ANISOU	3815	N	THR	A	582	2303	2377	2138	72	79	94	A	N
ATOM	3817	CA	THR	A	582	-5.927	29.340	12.201	1.00	19.48		A	C
ANISOU	3817	CA	THR	A	582	2408	2625	2366	3	49	45	A	C
ATOM	3819	CB	THR	A	582	-5.209	29.611	10.881	1.00	21.10		A	C
ANISOU	3819	CB	THR	A	582	2630	2797	2590	-61	76	67	A	C
ATOM	3821	OG1	THR	A	582	-4.405	28.471	10.600	1.00	24.39		A	O
ANISOU	3821	OG1	THR	A	582	3031	3298	2936	76	210	13	A	O
ATOM	3823	CG2	THR	A	582	-4.253	30.824	10.965	1.00	24.29		A	C
ANISOU	3823	CG2	THR	A	582	2961	3148	3120	-100	83	-1	A	C
ATOM	3827	C	THR	A	582	-6.581	30.616	12.699	1.00	18.71		A	C
ANISOU	3827	C	THR	A	582	2342	2443	2322	-74	45	124	A	C
ATOM	3828	O	THR	A	582	-6.087	31.274	13.607	1.00	18.37		A	O
ANISOU	3828	O	THR	A	582	2239	2615	2124	-109	70	280	A	O
ATOM	3829	N	ALA	A	583	-7.706	30.965	12.086	1.00	18.37		A	N
ANISOU	3829	N	ALA	A	583	2345	2455	2177	-4	3	192	A	N
ATOM	3831	CA	ALA	A	583	-8.422	32.164	12.474	1.00	18.86		A	C
ANISOU	3831	CA	ALA	A	583	2376	2444	2344	-10	-1	84	A	C
ATOM	3833	CB	ALA	A	583	-9.565	32.448	11.499	1.00	19.61		A	C
ANISOU	3833	CB	ALA	A	583	2481	2596	2374	4	-64	73	A	C
ATOM	3837	C	ALA	A	583	-8.995	32.046	13.875	1.00	18.34		A	C
ANISOU	3837	C	ALA	A	583	2329	2374	2265	31	-34	66	A	C
ATOM	3838	O	ALA	A	583	-8.982	33.003	14.621	1.00	19.83		A	O
ANISOU	3838	O	ALA	A	583	2620	2608	2304	39	5	108	A	O
ATOM	3839	N	MET	A	584	-9.502	30.863	14.217	1.00	17.49		A	N
ANISOU	3839	N	MET	A	584	2165	2267	2212	52	-3	36	A	N
ATOM	3841	CA	MET	A	584	-10.055	30.628	15.557	1.00	17.44		A	C
ANISOU	3841	CA	MET	A	584	2128	2259	2236	79	14	53	A	C

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ATOM	3843	CB	MET	A	584	-10.651	29.226	15.634	1.00	17.91		A	C
ANISOU	3843	CB	MET	A	584	2161	2376	2268	51	-7	-31	A	C
ATOM	3846	CG	MET	A	584	-11.063	28.765	16.984	1.00	18.66		A	C
ANISOU	3846	CG	MET	A	584	2299	2458	2332	11	-56	64	A	C
ATOM	3849	SD	MET	A	584	-11.627	27.011	16.949	1.00	19.54		A	S
ANISOU	3849	SD	MET	A	584	2272	2792	2359	-67	4	143	A	S
ATOM	3850	CE	MET	A	584	-11.783	26.771	18.710	1.00	18.97		A	C
ANISOU	3850	CE	MET	A	584	2282	2504	2420	-8	67	-22	A	C
ATOM	3854	C	MET	A	584	-8.968	30.788	16.601	1.00	16.98		A	C
ANISOU	3854	C	MET	A	584	2172	2162	2116	65	1	14	A	C
ATOM	3855	O	MET	A	584	-9.146	31.463	17.593	1.00	15.67		A	O
ANISOU	3855	O	MET	A	584	1936	1973	2044	196	39	91	A	O
ATOM	3856	N	LEU	A	585	-7.798	30.207	16.342	1.00	15.76		A	N
ANISOU	3856	N	LEU	A	585	1997	2025	1963	52	15	77	A	N
ATOM	3858	CA	LEU	A	585	-6.716	30.289	17.337	1.00	15.81		A	C
ANISOU	3858	CA	LEU	A	585	1976	2047	1981	34	16	11	A	C
ATOM	3860	CB	LEU	A	585	-5.570	29.351	16.973	1.00	15.98		A	C
ANISOU	3860	CB	LEU	A	585	1976	2164	1931	12	-2	10	A	C
ATOM	3863	CG	LEU	A	585	-6.015	27.898	16.913	1.00	17.14		A	C
ANISOU	3863	CG	LEU	A	585	2154	2262	2094	52	35	66	A	C
ATOM	3865	CD1	LEU	A	585	-4.884	27.118	16.233	1.00	18.14		A	C
ANISOU	3865	CD1	LEU	A	585	2220	2442	2228	98	38	-49	A	C
ATOM	3869	CD2	LEU	A	585	-6.336	27.303	18.273	1.00	16.01		A	C
ANISOU	3869	CD2	LEU	A	585	1830	2271	1979	64	8	74	A	C
ATOM	3873	C	LEU	A	585	-6.229	31.716	17.508	1.00	16.79		A	C
ANISOU	3873	C	LEU	A	585	2090	2192	2096	-12	-13	9	A	C
ATOM	3874	O	LEU	A	585	-5.927	32.142	18.615	1.00	16.36		A	O
ANISOU	3874	O	LEU	A	585	2052	2151	2012	-62	-22	-25	A	O
ATOM	3875	N	GLU	A	586	-6.147	32.459	16.400	1.00	17.47		A	N
ANISOU	3875	N	GLU	A	586	2221	2301	2113	-11	-66	37	A	N
ATOM	3877	CA	GLU	A	586	-5.686	33.845	16.444	1.00	18.96		A	C
ANISOU	3877	CA	GLU	A	586	2361	2423	2419	13	-11	64	A	C
ATOM	3879	CB	GLU	A	586	-5.433	34.366	15.030	1.00	19.41		A	C
ANISOU	3879	CB	GLU	A	586	2372	2570	2430	69	-25	81	A	C
ATOM	3882	CG	GLU	A	586	-4.837	35.776	15.054	1.00	23.85		A	C
ANISOU	3882	CG	GLU	A	586	3055	2923	3084	-12	-3	12	A	C
ATOM	3885	CD	GLU	A	586	-4.202	36.196	13.731	1.00	27.08		A	C
ANISOU	3885	CD	GLU	A	586	3514	3456	3317	-13	92	114	A	C
ATOM	3886	OE1	GLU	A	586	-3.475	35.391	13.122	1.00	27.65		A	O
ANISOU	3886	OE1	GLU	A	586	3758	3608	3140	32	12	93	A	O
ATOM	3887	OE2	GLU	A	586	-4.431	37.350	13.303	1.00	30.18		A	O
ANISOU	3887	OE2	GLU	A	586	3972	3615	3878	60	104	163	A	O
ATOM	3888	C	GLU	A	586	-6.665	34.749	17.182	1.00	19.00		A	C
ANISOU	3888	C	GLU	A	586	2502	2330	2385	36	-51	61	A	C
ATOM	3889	O	GLU	A	586	-6.271	35.783	17.734	1.00	20.01		A	O
ANISOU	3889	O	GLU	A	586	2635	2376	2590	-14	-68	63	A	O
ATOM	3890	N	LYS	A	587	-7.936	34.360	17.180	1.00	19.18		A	N
ANISOU	3890	N	LYS	A	587	2495	2356	2436	73	-63	68	A	N
ATOM	3892	CA	LYS	A	587	-8.972	35.058	17.936	1.00	20.33		A	C
ANISOU	3892	CA	LYS	A	587	2572	2513	2637	44	24	32	A	C
ATOM	3894	CB	LYS	A	587	-10.377	34.659	17.415	1.00	21.19		A	C
ANISOU	3894	CB	LYS	A	587	2662	2636	2753	65	5	-15	A	C
ATOM	3897	CG	ALYS	A	587	-10.699	35.243	16.051	0.50	23.27		A	C
ANISOU	3897	CG	ALYS	A	587	2957	2955	2928	20	-27	5	A	C
ATOM	3898	CG	BLYS	A	587	-10.749	35.199	16.067	0.50	24.05		A	C
ANISOU	3898	CG	BLYS	A	587	3095	3044	2997	14	-27	13	A	C
ATOM	3903	CD	ALYS	A	587	-11.916	34.608	15.403	0.50	23.99		A	C
ANISOU	3903	CD	ALYS	A	587	2980	3060	3075	42	-75	14	A	C
ATOM	3904	CD	BLYS	A	587	-12.221	34.973	15.790	0.50	26.25		A	C
ANISOU	3904	CD	BLYS	A	587	3205	3389	3377	6	-20	9	A	C
ATOM	3909	CE	ALYS	A	587	-13.172	34.816	16.239	0.50	24.39		A	C
ANISOU	3909	CE	ALYS	A	587	3095	3075	3095	-18	20	-3	A	C

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ATOM	3910	CE	BLYS	A	587	-12.469	34.637	14.318	0.50	28.33		A	C
ANISOU	3910	CE	BLYS	A	587	3655	3637	3470	-4	0	-24	A	C
ATOM	3915	NZ	ALYS	A	587	-14.331	33.990	15.746	0.50	23.65		A	N
ANISOU	3915	NZ	ALYS	A	587	2837	2941	3209	113	-84	58	A	N
ATOM	3916	NZ	BLYS	A	587	-12.311	33.192	13.984	0.50	29.21		A	N
ANISOU	3916	NZ	BLYS	A	587	3644	3697	3755	3	1	-13	A	N
ATOM	3923	C	LYS	A	587	-8.865	34.707	19.441	1.00	19.61		A	C
ANISOU	3923	C	LYS	A	587	2436	2493	2521	134	-55	-75	A	C
ATOM	3924	O	LYS	A	587	-9.655	35.152	20.273	1.00	21.20		A	O
ANISOU	3924	O	LYS	A	587	2494	2698	2862	220	-19	16	A	O
ATOM	3925	N	GLY	A	588	-7.907	33.859	19.805	1.00	18.97		A	N
ANISOU	3925	N	GLY	A	588	2464	2269	2474	78	-53	-10	A	N
ATOM	3927	CA	GLY	A	588	-7.751	33.469	21.182	1.00	18.15		A	C
ANISOU	3927	CA	GLY	A	588	2307	2284	2304	114	2	-63	A	C
ATOM	3930	C	GLY	A	588	-8.707	32.384	21.645	1.00	17.72		A	C
ANISOU	3930	C	GLY	A	588	2264	2260	2206	109	-21	-29	A	C
ATOM	3931	O	GLY	A	588	-8.839	32.135	22.851	1.00	19.45		A	O
ANISOU	3931	O	GLY	A	588	2533	2639	2215	92	68	-40	A	O
ATOM	3932	N	GLU	A	589	-9.346	31.689	20.704	1.00	15.55		A	N
ANISOU	3932	N	GLU	A	589	1995	1934	1980	186	-2	12	A	N
ATOM	3934	CA	GLU	A	589	-10.294	30.659	21.037	1.00	15.50		A	C
ANISOU	3934	CA	GLU	A	589	1987	1943	1957	147	29	-11	A	C
ATOM	3936	CB	GLU	A	589	-11.495	30.745	20.118	1.00	16.34		A	C
ANISOU	3936	CB	GLU	A	589	2024	2088	2093	42	81	43	A	C
ATOM	3939	CG	GLU	A	589	-12.324	31.984	20.394	1.00	18.89		A	C
ANISOU	3939	CG	GLU	A	589	2395	2312	2470	160	58	60	A	C
ATOM	3942	CD	GLU	A	589	-13.390	32.245	19.334	1.00	24.24		A	C
ANISOU	3942	CD	GLU	A	589	2979	3167	3064	120	-162	152	A	C
ATOM	3943	OE1	GLU	A	589	-13.660	31.356	18.490	1.00	26.92		A	O
ANISOU	3943	OE1	GLU	A	589	3278	3665	3286	300	-125	67	A	O
ATOM	3944	OE2	GLU	A	589	-13.997	33.340	19.428	1.00	27.57		A	O
ANISOU	3944	OE2	GLU	A	589	3299	3430	3746	335	73	186	A	O
ATOM	3945	C	GLU	A	589	-9.632	29.265	20.959	1.00	14.84		A	C
ANISOU	3945	C	GLU	A	589	1842	1832	1964	138	42	50	A	C
ATOM	3946	O	GLU	A	589	-8.694	29.068	20.202	1.00	14.39		A	O
ANISOU	3946	O	GLU	A	589	2019	1788	1661	211	112	188	A	O
ATOM	3947	N	ARG	A	590	-10.186	28.330	21.705	1.00	14.57		A	N
ANISOU	3947	N	ARG	A	590	1847	1847	1839	175	70	9	A	N
ATOM	3949	CA	ARG	A	590	-9.685	26.970	21.825	1.00	14.79		A	C
ANISOU	3949	CA	ARG	A	590	1879	1850	1888	70	-15	28	A	C
ATOM	3951	CB	ARG	A	590	-8.882	26.832	23.112	1.00	15.31		A	C
ANISOU	3951	CB	ARG	A	590	1935	1985	1895	51	13	53	A	C
ATOM	3954	CG	ARG	A	590	-7.687	27.777	23.228	1.00	14.46		A	C
ANISOU	3954	CG	ARG	A	590	1865	1778	1850	34	-134	-55	A	C
ATOM	3957	CD	ARG	A	590	-6.610	27.508	22.232	1.00	14.66		A	C
ANISOU	3957	CD	ARG	A	590	1773	1824	1971	69	-76	127	A	C
ATOM	3960	NE	ARG	A	590	-5.425	28.356	22.402	1.00	14.60		A	N
ANISOU	3960	NE	ARG	A	590	1670	1768	2110	99	-2	118	A	N
ATOM	3962	CZ	ARG	A	590	-5.204	29.508	21.790	1.00	15.88		A	C
ANISOU	3962	CZ	ARG	A	590	1855	1919	2257	93	-15	23	A	C
ATOM	3963	NH1	ARG	A	590	-6.087	30.013	20.924	1.00	15.24		A	N
ANISOU	3963	NH1	ARG	A	590	2054	1598	2137	22	39	151	A	N
ATOM	3966	NH2	ARG	A	590	-4.072	30.159	22.041	1.00	16.16		A	N
ANISOU	3966	NH2	ARG	A	590	2030	1764	2345	-51	3	99	A	N
ATOM	3969	C	ARG	A	590	-10.843	25.981	21.875	1.00	14.38		A	C
ANISOU	3969	C	ARG	A	590	1869	1857	1737	69	18	39	A	C
ATOM	3970	O	ARG	A	590	-11.950	26.343	22.261	1.00	15.16		A	O
ANISOU	3970	O	ARG	A	590	1889	2011	1859	87	-55	85	A	O
ATOM	3971	N	MET	A	591	-10.561	24.717	21.534	1.00	14.17		A	N
ANISOU	3971	N	MET	A	591	1831	1741	1811	39	43	93	A	N
ATOM	3973	CA	MET	A	591	-11.547	23.661	21.670	1.00	14.62		A	C
ANISOU	3973	CA	MET	A	591	1826	1902	1824	30	-21	-1	A	C

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ATOM	3975	CB	MET	A	591	-10.942	22.316	21.289	1.00	14.86		A	C
ANISOU	3975	CB	MET	A	591	1960	1854	1832	-4	62	66	A	C
ATOM	3978	CG	MET	A	591	-10.691	22.179	19.801	1.00	15.93		A	C
ANISOU	3978	CG	MET	A	591	2035	2050	1966	46	-3	24	A	C
ATOM	3981	SD	MET	A	591	-10.151	20.530	19.317	1.00	16.97		A	S
ANISOU	3981	SD	MET	A	591	2591	2032	1825	88	130	59	A	S
ATOM	3982	CE	MET	A	591	-8.467	20.483	19.972	1.00	17.54		A	C
ANISOU	3982	CE	MET	A	591	2398	2077	2189	-34	181	-21	A	C
ATOM	3986	C	MET	A	591	-12.051	23.620	23.099	1.00	15.76		A	C
ANISOU	3986	C	MET	A	591	2013	1960	2012	18	15	-6	A	C
ATOM	3987	O	MET	A	591	-11.308	23.832	24.040	1.00	15.58		A	O
ANISOU	3987	O	MET	A	591	1902	2004	2011	50	53	45	A	O
ATOM	3988	N	GLY	A	592	-13.341	23.341	23.246	1.00	17.01		A	N
ANISOU	3988	N	GLY	A	592	2030	2282	2151	56	4	-2	A	N
ATOM	3990	CA	GLY	A	592	-13.920	23.194	24.553	1.00	18.49		A	C
ANISOU	3990	CA	GLY	A	592	2246	2430	2349	14	71	-20	A	C
ATOM	3993	C	GLY	A	592	-13.498	21.935	25.259	1.00	19.16		A	C
ANISOU	3993	C	GLY	A	592	2334	2537	2407	1	76	17	A	C
ATOM	3994	O	GLY	A	592	-12.915	21.021	24.681	1.00	20.48		A	O
ANISOU	3994	O	GLY	A	592	2614	2690	2476	-15	198	30	A	O
ATOM	3995	N	CYS	A	593	-13.857	21.860	26.537	1.00	19.91		A	N
ANISOU	3995	N	CYS	A	593	2445	2663	2454	26	101	54	A	N
ATOM	3997	CA	CYS	A	593	-13.497	20.732	27.364	1.00	20.60		A	C
ANISOU	3997	CA	CYS	A	593	2415	2779	2631	62	74	49	A	C
ATOM	3999	CB	CYS	A	593	-13.784	21.106	28.811	1.00	21.52		A	C
ANISOU	3999	CB	CYS	A	593	2596	2898	2680	34	67	-24	A	C
ATOM	4002	SG	CYS	A	593	-13.289	19.808	29.947	1.00	24.11		A	S
ANISOU	4002	SG	CYS	A	593	2626	3482	3050	63	300	243	A	S
ATOM	4003	C	CYS	A	593	-14.324	19.528	26.988	1.00	20.11		A	C
ANISOU	4003	C	CYS	A	593	2448	2651	2541	42	60	103	A	C
ATOM	4004	O	CYS	A	593	-15.570	19.630	26.949	1.00	20.56		A	O
ANISOU	4004	O	CYS	A	593	2281	2760	2767	21	62	174	A	O
ATOM	4005	N	PRO	A	594	-13.705	18.389	26.702	1.00	20.81		A	N
ANISOU	4005	N	PRO	A	594	2467	2766	2673	42	21	89	A	N
ATOM	4006	CA	PRO	A	594	-14.486	17.195	26.358	1.00	21.10		A	C
ANISOU	4006	CA	PRO	A	594	2592	2707	2714	42	67	91	A	C
ATOM	4008	CB	PRO	A	594	-13.418	16.127	26.051	1.00	21.40		A	C
ANISOU	4008	CB	PRO	A	594	2611	2769	2750	10	25	13	A	C
ATOM	4011	CG	PRO	A	594	-12.146	16.916	25.773	1.00	22.11		A	C
ANISOU	4011	CG	PRO	A	594	2688	2782	2931	9	155	113	A	C
ATOM	4014	CD	PRO	A	594	-12.244	18.156	26.627	1.00	21.07		A	C
ANISOU	4014	CD	PRO	A	594	2532	2773	2698	13	66	112	A	C
ATOM	4017	C	PRO	A	594	-15.383	16.759	27.529	1.00	22.09		A	C
ANISOU	4017	C	PRO	A	594	2703	2880	2810	-27	73	48	A	C
ATOM	4018	O	PRO	A	594	-15.072	17.032	28.697	1.00	21.86		A	O
ANISOU	4018	O	PRO	A	594	2403	3033	2867	-27	90	247	A	O
ATOM	4019	N	ALA	A	595	-16.535	16.208	27.177	1.00	23.39		A	N
ANISOU	4019	N	ALA	A	595	2881	3023	2983	-29	43	86	A	N
ATOM	4021	CA	ALA	A	595	-17.470	15.671	28.162	1.00	23.76		A	C
ANISOU	4021	CA	ALA	A	595	2915	3067	3044	-42	58	21	A	C
ATOM	4023	CB	ALA	A	595	-18.569	14.924	27.460	1.00	24.41		A	C
ANISOU	4023	CB	ALA	A	595	3041	3141	3090	-72	44	15	A	C
ATOM	4027	C	ALA	A	595	-16.732	14.731	29.096	1.00	24.26		A	C
ANISOU	4027	C	ALA	A	595	2983	3106	3127	-56	33	23	A	C
ATOM	4028	O	ALA	A	595	-16.063	13.805	28.637	1.00	24.68		A	O
ANISOU	4028	O	ALA	A	595	2830	3275	3269	-40	171	119	A	O
ATOM	4029	N	GLY	A	596	-16.839	14.986	30.392	1.00	24.54		A	N
ANISOU	4029	N	GLY	A	596	2934	3252	3136	-38	70	103	A	N
ATOM	4031	CA	GLY	A	596	-16.254	14.114	31.399	1.00	25.07		A	C
ANISOU	4031	CA	GLY	A	596	3077	3221	3225	-6	46	110	A	C
ATOM	4034	C	GLY	A	596	-14.757	14.222	31.582	1.00	25.21		A	C
ANISOU	4034	C	GLY	A	596	3081	3247	3248	-3	42	158	A	C



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ATOM	4035	O	GLY A 596	-14.156	13.461	32.343	1.00	26.92		A	O
ANISOU	4035	O	GLY A 596	3291	3508	3427	10	110	376	A	O
ATOM	4036	N	CYS A 597	-14.131	15.169	30.895	1.00	24.58		A	N
ANISOU	4036	N	CYS A 597	2954	3201	3183	-13	80	158	A	N
ATOM	4038	CA	CYS A 597	-12.683	15.307	31.003	1.00	23.41		A	C
ANISOU	4038	CA	CYS A 597	2847	3022	3026	20	80	121	A	C
ATOM	4040	CB	CYS A 597	-12.136	16.128	29.838	1.00	22.58		A	C
ANISOU	4040	CB	CYS A 597	2596	3018	2964	26	140	93	A	C
ATOM	4043	SG	CYS A 597	-10.344	16.460	29.874	1.00	21.69		A	S
ANISOU	4043	SG	CYS A 597	2185	3139	2916	24	448	333	A	S
ATOM	4044	C	CYS A 597	-12.363	15.974	32.319	1.00	22.90		A	C
ANISOU	4044	C	CYS A 597	2790	2891	3019	-45	120	72	A	C
ATOM	4045	O	CYS A 597	-12.986	16.986	32.658	1.00	23.90		A	O
ANISOU	4045	O	CYS A 597	3000	2958	3122	-10	187	135	A	O
ATOM	4046	N	PRO A 598	-11.435	15.418	33.090	1.00	22.68		A	N
ANISOU	4046	N	PRO A 598	2868	2849	2900	-37	153	64	A	N
ATOM	4047	CA	PRO A 598	-11.023	16.038	34.345	1.00	22.63		A	C
ANISOU	4047	CA	PRO A 598	2821	2851	2923	-26	85	31	A	C
ATOM	4049	CB	PRO A 598	-9.885	15.144	34.844	1.00	23.33		A	C
ANISOU	4049	CB	PRO A 598	2983	2890	2990	-57	89	95	A	C
ATOM	4052	CG	PRO A 598	-9.989	13.914	34.071	1.00	23.47		A	C
ANISOU	4052	CG	PRO A 598	2979	2994	2942	36	136	6	A	C
ATOM	4055	CD	PRO A 598	-10.698	14.180	32.826	1.00	22.69		A	C
ANISOU	4055	CD	PRO A 598	2802	2849	2969	-23	90	42	A	C
ATOM	4058	C	PRO A 598	-10.529	17.455	34.140	1.00	22.53		A	C
ANISOU	4058	C	PRO A 598	2883	2838	2839	-6	105	58	A	C
ATOM	4059	O	PRO A 598	-9.812	17.732	33.169	1.00	20.67		A	O
ANISOU	4059	O	PRO A 598	2488	2627	2738	49	298	34	A	O
ATOM	4060	N	ARG A 599	-10.891	18.353	35.049	1.00	22.01		A	N
ANISOU	4060	N	ARG A 599	2763	2794	2803	20	189	17	A	N
ATOM	4062	CA	ARG A 599	-10.486	19.753	34.899	1.00	23.45		A	C
ANISOU	4062	CA	ARG A 599	2984	2930	2993	10	70	-6	A	C
ATOM	4064	CB	ARG A 599	-11.026	20.581	36.074	1.00	24.62		A	C
ANISOU	4064	CB	ARG A 599	3134	3141	3077	28	92	-33	A	C
ATOM	4067	CG	ARG A 599	-10.859	22.082	35.912	1.00	28.15		A	C
ANISOU	4067	CG	ARG A 599	3620	3457	3619	-8	20	-57	A	C
ATOM	4070	CD	ARG A 599	-11.246	22.627	34.545	1.00	31.55		A	C
ANISOU	4070	CD	ARG A 599	4183	3917	3888	34	12	57	A	C
ATOM	4073	NE	ARG A 599	-12.591	22.246	34.124	1.00	34.74		A	N
ANISOU	4073	NE	ARG A 599	4335	4389	4475	-9	75	13	A	N
ATOM	4075	CZ	ARG A 599	-13.128	22.553	32.951	1.00	37.87		A	C
ANISOU	4075	CZ	ARG A 599	4827	4807	4752	16	-40	31	A	C
ATOM	4076	NH1	ARG A 599	-12.428	23.254	32.065	1.00	39.84		A	N
ANISOU	4076	NH1	ARG A 599	5060	5073	5001	-1	45	109	A	N
ATOM	4079	NH2	ARG A 599	-14.363	22.158	32.652	1.00	38.75		A	N
ANISOU	4079	NH2	ARG A 599	4836	4951	4936	22	0	11	A	N
ATOM	4082	C	ARG A 599	-8.975	19.930	34.786	1.00	22.04		A	C
ANISOU	4082	C	ARG A 599	2868	2744	2759	23	84	30	A	C
ATOM	4083	O	ARG A 599	-8.482	20.767	34.029	1.00	20.98		A	O
ANISOU	4083	O	ARG A 599	2788	2552	2631	118	199	190	A	O
ATOM	4084	N	GLU A 600	-8.224	19.132	35.528	1.00	21.42		A	N
ANISOU	4084	N	GLU A 600	2811	2685	2642	20	101	30	A	N
ATOM	4086	CA	GLU A 600	-6.785	19.255	35.541	1.00	21.36		A	C
ANISOU	4086	CA	GLU A 600	2795	2687	2632	31	24	-19	A	C
ATOM	4088	CB	GLU A 600	-6.191	18.304	36.580	1.00	22.89		A	C
ANISOU	4088	CB	GLU A 600	2999	2847	2849	66	52	32	A	C
ATOM	4091	CG	GLU A 600	-6.460	18.703	38.027	1.00	27.32		A	C
ANISOU	4091	CG	GLU A 600	3633	3530	3217	45	-16	-56	A	C
ATOM	4094	CD	GLU A 600	-7.754	18.114	38.604	1.00	30.88		A	C
ANISOU	4094	CD	GLU A 600	3889	3995	3848	-67	58	56	A	C
ATOM	4095	OE1	GLU A 600	-8.657	17.648	37.847	1.00	30.57		A	O
ANISOU	4095	OE1	GLU A 600	4054	4058	3500	-65	61	121	A	O

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ATOM	4096	OE2	GLU	A	600	-7.882	18.121	39.857	1.00	34.92		A	O
ANISOU	4096	OE2	GLU	A	600	4682	4550	4036	1	7	-4	A	O
ATOM	4097	C	GLU	A	600	-6.191	18.946	34.170	1.00	19.18		A	C
ANISOU	4097	C	GLU	A	600	2489	2391	2407	20	10	71	A	C
ATOM	4098	O	GLU	A	600	-5.186	19.544	33.781	1.00	17.92		A	O
ANISOU	4098	O	GLU	A	600	2410	2281	2116	34	51	17	A	O
ATOM	4099	N	MET	A	601	-6.802	17.996	33.463	1.00	17.56		A	N
ANISOU	4099	N	MET	A	601	2316	2237	2116	68	45	120	A	N
ATOM	4101	CA	MET	A	601	-6.335	17.631	32.131	1.00	17.09		A	C
ANISOU	4101	CA	MET	A	601	2147	2194	2150	96	39	104	A	C
ATOM	4103	CB	MET	A	601	-6.873	16.291	31.708	1.00	17.45		A	C
ANISOU	4103	CB	MET	A	601	2251	2245	2133	109	45	164	A	C
ATOM	4106	CG	AMET	A	601	-6.290	15.149	32.559	0.50	17.23		A	C
ANISOU	4106	CG	AMET	A	601	2277	2084	2184	42	59	140	A	C
ATOM	4107	CG	BMET	A	601	-6.359	15.120	32.545	0.50	16.87		A	C
ANISOU	4107	CG	BMET	A	601	2197	2061	2152	50	68	131	A	C
ATOM	4112	SD	AMET	A	601	-4.476	15.051	32.545	0.50	18.28		A	S
ANISOU	4112	SD	AMET	A	601	2309	2276	2359	172	275	243	A	S
ATOM	4113	SD	BMET	A	601	-4.593	14.834	32.474	0.50	17.41		A	S
ANISOU	4113	SD	BMET	A	601	2173	2180	2260	183	283	282	A	S
ATOM	4114	CE	AMET	A	601	-4.003	16.171	33.774	0.50	19.34		A	C
ANISOU	4114	CE	AMET	A	601	2512	2442	2393	39	78	170	A	C
ATOM	4115	CE	BMET	A	601	-4.286	14.735	30.803	0.50	17.95		A	C
ANISOU	4115	CE	BMET	A	601	2230	2327	2261	-18	-9	7	A	C
ATOM	4122	C	MET	A	601	-6.687	18.727	31.136	1.00	16.46		A	C
ANISOU	4122	C	MET	A	601	2041	2095	2118	43	93	134	A	C
ATOM	4123	O	MET	A	601	-5.889	19.027	30.255	1.00	16.52		A	O
ANISOU	4123	O	MET	A	601	2069	2073	2134	154	232	208	A	O
ATOM	4124	N	TYR	A	602	-7.884	19.308	31.233	1.00	16.07		A	N
ANISOU	4124	N	TYR	A	602	2007	2030	2068	110	134	184	A	N
ATOM	4126	CA	TYR	A	602	-8.200	20.419	30.335	1.00	16.22		A	C
ANISOU	4126	CA	TYR	A	602	2033	2096	2031	69	46	153	A	C
ATOM	4128	CB	TYR	A	602	-9.678	20.848	30.360	1.00	17.47		A	C
ANISOU	4128	CB	TYR	A	602	2216	2183	2238	115	56	124	A	C
ATOM	4131	CG	TYR	A	602	-9.894	21.860	29.260	1.00	19.23		A	C
ANISOU	4131	CG	TYR	A	602	2486	2510	2309	85	-1	209	A	C
ATOM	4132	CD1	TYR	A	602	-10.073	21.450	27.940	1.00	18.38		A	C
ANISOU	4132	CD1	TYR	A	602	2253	2342	2389	-22	-30	24	A	C
ATOM	4134	CE1	TYR	A	602	-10.173	22.406	26.883	1.00	19.08		A	C
ANISOU	4134	CE1	TYR	A	602	2394	2321	2535	115	49	120	A	C
ATOM	4136	CZ	TYR	A	602	-10.014	23.757	27.170	1.00	20.38		A	C
ANISOU	4136	CZ	TYR	A	602	2596	2577	2568	104	2	20	A	C
ATOM	4137	OH	TYR	A	602	-10.081	24.712	26.163	1.00	22.61		A	O
ANISOU	4137	OH	TYR	A	602	3134	2679	2777	178	-63	32	A	O
ATOM	4139	CE2	TYR	A	602	-9.788	24.163	28.456	1.00	21.37		A	C
ANISOU	4139	CE2	TYR	A	602	2891	2553	2673	5	-35	-7	A	C
ATOM	4141	CD2	TYR	A	602	-9.698	23.207	29.495	1.00	21.61		A	C
ANISOU	4141	CD2	TYR	A	602	2943	2734	2532	128	-40	18	A	C
ATOM	4143	C	TYR	A	602	-7.283	21.611	30.624	1.00	16.13		A	C
ANISOU	4143	C	TYR	A	602	2038	2053	2038	134	29	77	A	C
ATOM	4144	O	TYR	A	602	-6.808	22.297	29.701	1.00	15.92		A	O
ANISOU	4144	O	TYR	A	602	2144	2078	1826	52	116	169	A	O
ATOM	4145	N	ASP	A	603	-7.007	21.883	31.886	1.00	15.51		A	N
ANISOU	4145	N	ASP	A	603	2018	2015	1858	158	111	110	A	N
ATOM	4147	CA	ASP	A	603	-6.103	22.970	32.233	1.00	16.46		A	C
ANISOU	4147	CA	ASP	A	603	2149	2106	1997	68	61	63	A	C
ATOM	4149	CB	ASP	A	603	-5.808	22.995	33.715	1.00	17.68		A	C
ANISOU	4149	CB	ASP	A	603	2339	2308	2068	85	50	-36	A	C
ATOM	4152	CG	ASP	A	603	-6.957	23.499	34.580	1.00	20.46		A	C
ANISOU	4152	CG	ASP	A	603	2614	2706	2453	42	100	-33	A	C
ATOM	4153	OD1	ASP	A	603	-7.944	24.054	34.097	1.00	22.98		A	O
ANISOU	4153	OD1	ASP	A	603	2930	3118	2681	157	161	-62	A	O

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ATOM	4154	OD2	ASP	A	603	-6.909	23.288	35.826	1.00	26.17		A	O
ANISOU	4154	OD2	ASP	A	603	3680	3636	2627	-66	355	35	A	O
ATOM	4155	C	ASP	A	603	-4.746	22.775	31.528	1.00	15.50		A	C
ANISOU	4155	C	ASP	A	603	2015	1966	1909	34	-10	32	A	C
ATOM	4156	O	ASP	A	603	-4.149	23.707	30.961	1.00	15.65		A	O
ANISOU	4156	O	ASP	A	603	2036	2049	1860	-47	0	35	A	O
ATOM	4157	N	LEU	A	604	-4.254	21.543	31.561	1.00	15.40		A	N
ANISOU	4157	N	LEU	A	604	2005	1928	1918	21	45	110	A	N
ATOM	4159	CA	LEU	A	604	-2.998	21.248	30.922	1.00	15.54		A	C
ANISOU	4159	CA	LEU	A	604	1987	1986	1930	42	24	19	A	C
ATOM	4161	CB	LEU	A	604	-2.541	19.833	31.253	1.00	16.18		A	C
ANISOU	4161	CB	LEU	A	604	2099	2078	1970	31	-2	90	A	C
ATOM	4164	CG	LEU	A	604	-1.143	19.472	30.769	1.00	17.98		A	C
ANISOU	4164	CG	LEU	A	604	2293	2224	2314	53	87	-5	A	C
ATOM	4166	CD1	LEU	A	604	-0.065	20.451	31.251	1.00	19.12		A	C
ANISOU	4166	CD1	LEU	A	604	2373	2353	2537	-4	36	-12	A	C
ATOM	4170	CD2	LEU	A	604	-0.800	18.018	31.231	1.00	18.43		A	C
ANISOU	4170	CD2	LEU	A	604	2482	2349	2169	175	25	105	A	C
ATOM	4174	C	LEU	A	604	-3.081	21.446	29.404	1.00	14.39		A	C
ANISOU	4174	C	LEU	A	604	1792	1877	1798	24	27	61	A	C
ATOM	4175	O	LEU	A	604	-2.137	21.971	28.811	1.00	14.58		A	O
ANISOU	4175	O	LEU	A	604	1736	1923	1877	94	83	79	A	O
ATOM	4176	N	MET	A	605	-4.179	21.015	28.778	1.00	14.35		A	N
ANISOU	4176	N	MET	A	605	1783	1928	1742	42	79	14	A	N
ATOM	4178	CA	MET	A	605	-4.331	21.211	27.343	1.00	14.51		A	C
ANISOU	4178	CA	MET	A	605	1814	1871	1828	-23	0	-6	A	C
ATOM	4180	CB	MET	A	605	-5.702	20.746	26.873	1.00	15.48		A	C
ANISOU	4180	CB	MET	A	605	1914	2064	1903	-56	-26	43	A	C
ATOM	4183	CG	MET	A	605	-5.854	19.287	26.859	1.00	15.58		A	C
ANISOU	4183	CG	MET	A	605	1970	2019	1929	130	-24	9	A	C
ATOM	4186	SD	MET	A	605	-7.632	18.917	26.513	1.00	17.87		A	S
ANISOU	4186	SD	MET	A	605	2025	2441	2324	-33	83	-186	A	S
ATOM	4187	CE	MET	A	605	-7.709	17.342	27.354	1.00	17.92		A	C
ANISOU	4187	CE	MET	A	605	1934	2662	2213	-125	247	121	A	C
ATOM	4191	C	MET	A	605	-4.208	22.691	27.027	1.00	15.17		A	C
ANISOU	4191	C	MET	A	605	1977	1934	1852	29	25	20	A	C
ATOM	4192	O	MET	A	605	-3.527	23.076	26.096	1.00	15.01		A	O
ANISOU	4192	O	MET	A	605	1983	1965	1752	9	88	120	A	O
ATOM	4193	N	ASN	A	606	-4.874	23.531	27.807	1.00	14.83		A	N
ANISOU	4193	N	ASN	A	606	1913	1913	1808	56	103	-6	A	N
ATOM	4195	CA	ASN	A	606	-4.845	24.965	27.531	1.00	15.93		A	C
ANISOU	4195	CA	ASN	A	606	2060	2027	1966	56	86	-4	A	C
ATOM	4197	CB	ASN	A	606	-5.821	25.678	28.454	1.00	17.38		A	C
ANISOU	4197	CB	ASN	A	606	2232	2247	2125	50	123	-26	A	C
ATOM	4200	CG	AASN	A	606	-7.148	26.029	27.790	0.50	19.93		A	C
ANISOU	4200	CG	AASN	A	606	2474	2643	2455	60	5	-11	A	C
ATOM	4201	CG	BASN	A	606	-6.073	27.126	28.014	0.50	16.45		A	C
ANISOU	4201	CG	BASN	A	606	2022	2158	2068	47	121	-40	A	C
ATOM	4202	OD1AASN	A	606	-7.235	26.364	26.611	0.50	21.26		A	O	
ANISOU	4202	OD1AASN	A	606	2745	2702	2628	48	-38	128	A	O	
ATOM	4203	OD1BASN	A	606	-6.660	27.374	26.987	0.50	19.03		A	O	
ANISOU	4203	OD1BASN	A	606	2533	2264	2434	128	-33	1	A	O	
ATOM	4204	ND2AASN	A	606	-8.223	25.837	28.551	0.50	25.57		A	N	
ANISOU	4204	ND2AASN	A	606	3048	3502	3164	-107	94	154	A	N	
ATOM	4205	ND2BASN	A	606	-5.504	28.078	28.754	0.50	17.04		A	N	
ANISOU	4205	ND2BASN	A	606	2059	2353	2062	74	290	41	A	N	
ATOM	4210	C	ASN	A	606	-3.475	25.562	27.681	1.00	15.64		A	C
ANISOU	4210	C	ASN	A	606	2025	1934	1982	75	88	24	A	C
ATOM	4211	O	ASN	A	606	-3.092	26.458	26.936	1.00	17.10		A	O
ANISOU	4211	O	ASN	A	606	2156	1969	2371	119	150	208	A	O
ATOM	4212	N	LEU	A	607	-2.725	25.100	28.670	1.00	15.26		A	N
ANISOU	4212	N	LEU	A	607	1953	1914	1930	26	82	73	A	N

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ATOM	4214	CA	LEU	A	607	-1.353	25.542	28.825	1.00	15.69		A	C
ANISOU	4214	CA	LEU	A	607	2013	1969	1977	9	-3	66	A	C
ATOM	4216	CB	LEU	A	607	-0.779	24.897	30.066	1.00	17.19		A	C
ANISOU	4216	CB	LEU	A	607	2221	2191	2118	22	-9	50	A	C
ATOM	4219	CG	ALEU	A	607	-1.065	25.485	31.449	0.60	17.71		A	C
ANISOU	4219	CG	ALEU	A	607	2200	2298	2230	24	37	6	A	C
ATOM	4220	CG	BLEU	A	607	0.407	25.492	30.826	0.40	18.62		A	C
ANISOU	4220	CG	BLEU	A	607	2285	2370	2418	10	5	13	A	C
ATOM	4223	CD1	ALEU	A	607	-0.497	24.633	32.577	0.60	18.23		A	C
ANISOU	4223	CD1	ALEU	A	607	2297	2341	2287	-32	16	28	A	C
ATOM	4224	CD1	BLEU	A	607	0.283	26.968	31.137	0.40	20.04		A	C
ANISOU	4224	CD1	BLEU	A	607	2512	2498	2602	-34	16	-44	A	C
ATOM	4231	CD2	ALEU	A	607	-0.734	26.938	31.568	0.60	20.62		A	C
ANISOU	4231	CD2	ALEU	A	607	2628	2497	2710	-8	65	-84	A	C
ATOM	4232	CD2	BLEU	A	607	0.753	24.684	32.068	0.40	19.49		A	C
ANISOU	4232	CD2	BLEU	A	607	2428	2519	2456	39	-23	34	A	C
ATOM	4239	C	LEU	A	607	-0.538	25.145	27.578	1.00	14.63		A	C
ANISOU	4239	C	LEU	A	607	1833	1803	1921	39	-23	31	A	C
ATOM	4240	O	LEU	A	607	0.246	25.944	27.072	1.00	14.79		A	O
ANISOU	4240	O	LEU	A	607	1895	1770	1954	5	1	10	A	O
ATOM	4241	N	CYS	A	608	-0.721	23.919	27.070	1.00	13.35		A	N
ANISOU	4241	N	CYS	A	608	1682	1714	1674	34	7	15	A	N
ATOM	4243	CA	CYS	A	608	-0.028	23.498	25.869	1.00	12.76		A	C
ANISOU	4243	CA	CYS	A	608	1543	1655	1650	60	1	71	A	C
ATOM	4245	CB	CYS	A	608	-0.335	22.054	25.533	1.00	12.92		A	C
ANISOU	4245	CB	CYS	A	608	1478	1788	1643	25	-92	10	A	C
ATOM	4248	SG	CYS	A	608	0.312	20.833	26.708	1.00	15.04		A	S
ANISOU	4248	SG	CYS	A	608	1878	1857	1976	-22	7	226	A	S
ATOM	4249	C	CYS	A	608	-0.382	24.364	24.678	1.00	13.55		A	C
ANISOU	4249	C	CYS	A	608	1713	1736	1699	52	53	44	A	C
ATOM	4250	O	CYS	A	608	0.448	24.550	23.790	1.00	14.35		A	O
ANISOU	4250	O	CYS	A	608	1705	1865	1881	1	55	30	A	O
ATOM	4251	N	TRP	A	609	-1.605	24.914	24.684	1.00	12.76		A	N
ANISOU	4251	N	TRP	A	609	1582	1676	1587	12	-38	39	A	N
ATOM	4253	CA	TRP	A	609	-2.063	25.777	23.601	1.00	12.58		A	C
ANISOU	4253	CA	TRP	A	609	1560	1587	1631	27	4	47	A	C
ATOM	4255	CB	TRP	A	609	-3.543	25.546	23.314	1.00	13.21		A	C
ANISOU	4255	CB	TRP	A	609	1654	1628	1736	23	-54	46	A	C
ATOM	4258	CG	TRP	A	609	-3.927	24.162	22.947	1.00	12.95		A	C
ANISOU	4258	CG	TRP	A	609	1567	1653	1699	-55	8	-31	A	C
ATOM	4259	CD1	TRP	A	609	-3.196	23.243	22.240	1.00	12.62		A	C
ANISOU	4259	CD1	TRP	A	609	1334	1806	1654	1	22	54	A	C
ATOM	4261	NE1	TRP	A	609	-3.907	22.074	22.105	1.00	12.49		A	N
ANISOU	4261	NE1	TRP	A	609	1434	1737	1572	103	-64	-15	A	N
ATOM	4263	CE2	TRP	A	609	-5.139	22.238	22.692	1.00	12.94		A	C
ANISOU	4263	CE2	TRP	A	609	1502	1649	1765	102	88	-56	A	C
ATOM	4264	CD2	TRP	A	609	-5.172	23.527	23.248	1.00	11.94		A	C
ANISOU	4264	CD2	TRP	A	609	1416	1501	1618	-13	-61	22	A	C
ATOM	4265	CE3	TRP	A	609	-6.324	23.927	23.933	1.00	13.13		A	C
ANISOU	4265	CE3	TRP	A	609	1579	1715	1694	25	62	73	A	C
ATOM	4267	CZ3	TRP	A	609	-7.366	23.058	24.044	1.00	12.78		A	C
ANISOU	4267	CZ3	TRP	A	609	1497	1727	1630	37	139	-19	A	C
ATOM	4269	CH2	TRP	A	609	-7.316	21.801	23.485	1.00	13.99		A	C
ANISOU	4269	CH2	TRP	A	609	1852	1586	1877	-101	166	169	A	C
ATOM	4271	CZ2	TRP	A	609	-6.206	21.350	22.827	1.00	13.78		A	C
ANISOU	4271	CZ2	TRP	A	609	1544	1792	1899	85	-5	-53	A	C
ATOM	4273	C	TRP	A	609	-1.810	27.267	23.860	1.00	13.72		A	C
ANISOU	4273	C	TRP	A	609	1681	1715	1814	43	-18	-17	A	C
ATOM	4274	O	TRP	A	609	-2.516	28.140	23.352	1.00	14.57		A	O
ANISOU	4274	O	TRP	A	609	1770	1765	2000	39	-97	114	A	O
ATOM	4275	N	THR	A	610	-0.761	27.570	24.604	1.00	12.90		A	N
ANISOU	4275	N	THR	A	610	1625	1492	1785	-24	-65	30	A	N

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ATOM	4277	CA	THR	A	610	-0.342	28.954	24.793	1.00	13.75		A	C
ANISOU	4277	CA	THR	A	610	1788	1585	1850	82	58	-65	A	C
ATOM	4279	CB	THR	A	610	0.756	28.974	25.831	1.00	14.35		A	C
ANISOU	4279	CB	THR	A	610	1906	1698	1848	6	31	-43	A	C
ATOM	4281	OG1	THR	A	610	0.227	28.616	27.117	1.00	16.43		A	O
ANISOU	4281	OG1	THR	A	610	2329	1921	1991	-22	45	38	A	O
ATOM	4283	CG2	THR	A	610	1.372	30.332	25.990	1.00	15.19		A	C
ANISOU	4283	CG2	THR	A	610	1923	1803	2045	83	-8	-54	A	C
ATOM	4287	C	THR	A	610	0.163	29.489	23.464	1.00	13.61		A	C
ANISOU	4287	C	THR	A	610	1786	1567	1817	23	22	3	A	C
ATOM	4288	O	THR	A	610	1.028	28.872	22.811	1.00	13.90		A	O
ANISOU	4288	O	THR	A	610	1814	1538	1926	100	46	37	A	O
ATOM	4289	N	TYR	A	611	-0.369	30.630	23.037	1.00	14.90		A	N
ANISOU	4289	N	TYR	A	611	1944	1816	1900	77	42	0	A	N
ATOM	4291	CA	TYR	A	611	-0.003	31.196	21.754	1.00	14.20		A	C
ANISOU	4291	CA	TYR	A	611	1770	1718	1905	-2	56	34	A	C
ATOM	4293	CB	TYR	A	611	-0.876	32.448	21.452	1.00	14.48		A	C
ANISOU	4293	CB	TYR	A	611	1816	1775	1910	-19	64	27	A	C
ATOM	4296	CG	TYR	A	611	-0.736	32.946	20.051	1.00	14.48		A	C
ANISOU	4296	CG	TYR	A	611	1858	1639	2004	84	-25	37	A	C
ATOM	4297	CD1	TYR	A	611	0.318	33.784	19.689	1.00	17.04		A	C
ANISOU	4297	CD1	TYR	A	611	2108	2089	2276	16	55	65	A	C
ATOM	4299	CE1	TYR	A	611	0.457	34.223	18.384	1.00	17.14		A	C
ANISOU	4299	CE1	TYR	A	611	2194	2043	2272	82	-2	94	A	C
ATOM	4301	CZ	TYR	A	611	-0.469	33.839	17.423	1.00	16.27		A	C
ANISOU	4301	CZ	TYR	A	611	2097	1893	2192	80	-1	-7	A	C
ATOM	4302	OH	TYR	A	611	-0.327	34.270	16.117	1.00	18.31		A	O
ANISOU	4302	OH	TYR	A	611	2212	2289	2455	179	61	159	A	O
ATOM	4304	CE2	TYR	A	611	-1.527	33.024	17.760	1.00	16.23		A	C
ANISOU	4304	CE2	TYR	A	611	2090	1980	2097	122	-64	141	A	C
ATOM	4306	CD2	TYR	A	611	-1.633	32.565	19.077	1.00	14.50		A	C
ANISOU	4306	CD2	TYR	A	611	1754	1871	1883	16	95	10	A	C
ATOM	4308	C	TYR	A	611	1.495	31.568	21.697	1.00	15.42		A	C
ANISOU	4308	C	TYR	A	611	1892	1876	2089	79	43	95	A	C
ATOM	4309	O	TYR	A	611	2.173	31.204	20.744	1.00	17.42		A	O
ANISOU	4309	O	TYR	A	611	2123	2033	2461	127	102	253	A	O
ATOM	4310	N	ASP	A	612	1.960	32.284	22.712	1.00	17.45		A	N
ANISOU	4310	N	ASP	A	612	2101	2150	2377	61	21	57	A	N
ATOM	4312	CA	ASP	A	612	3.328	32.779	22.793	1.00	19.55		A	C
ANISOU	4312	CA	ASP	A	612	2382	2471	2573	14	11	76	A	C
ATOM	4314	CB	ASP	A	612	3.441	33.777	23.932	1.00	20.74		A	C
ANISOU	4314	CB	ASP	A	612	2595	2588	2697	29	-32	72	A	C
ATOM	4317	CG	ASP	A	612	4.813	34.345	24.048	1.00	25.12		A	C
ANISOU	4317	CG	ASP	A	612	3006	3229	3306	-106	-25	42	A	C
ATOM	4318	OD1	ASP	A	612	5.236	35.091	23.138	1.00	28.21		A	O
ANISOU	4318	OD1	ASP	A	612	3496	3550	3674	-207	66	152	A	O
ATOM	4319	OD2	ASP	A	612	5.544	34.057	24.990	1.00	28.97		A	O
ANISOU	4319	OD2	ASP	A	612	3394	3867	3746	-72	-238	46	A	O
ATOM	4320	C	ASP	A	612	4.281	31.630	23.058	1.00	20.15		A	C
ANISOU	4320	C	ASP	A	612	2529	2497	2627	45	16	76	A	C
ATOM	4321	O	ASP	A	612	4.162	30.933	24.061	1.00	20.39		A	O
ANISOU	4321	O	ASP	A	612	2448	2550	2746	87	23	247	A	O
ATOM	4322	N	VAL	A	613	5.238	31.452	22.174	1.00	21.72		A	N
ANISOU	4322	N	VAL	A	613	2667	2715	2870	81	12	106	A	N
ATOM	4324	CA	VAL	A	613	6.180	30.348	22.284	1.00	22.71		A	C
ANISOU	4324	CA	VAL	A	613	2792	2825	3008	43	-22	54	A	C
ATOM	4326	CB	VAL	A	613	7.175	30.419	21.154	1.00	23.85		A	C
ANISOU	4326	CB	VAL	A	613	2986	3026	3049	87	-2	12	A	C
ATOM	4328	CG1	VAL	A	613	8.334	29.425	21.384	1.00	24.95		A	C
ANISOU	4328	CG1	VAL	A	613	2991	3241	3246	64	4	-7	A	C
ATOM	4332	CG2	VAL	A	613	6.482	30.189	19.824	1.00	24.91		A	C
ANISOU	4332	CG2	VAL	A	613	3067	3250	3147	3	74	-14	A	C

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ATOM	4336	C	VAL	A	613	6.912	30.399	23.617	1.00	22.87		A	C
ANISOU	4336	C	VAL	A	613	2794	2894	3002	10	2	34	A	C
ATOM	4337	O	VAL	A	613	7.073	29.380	24.297	1.00	21.86		A	O
ANISOU	4337	O	VAL	A	613	2340	2816	3149	-25	-24	109	A	O
ATOM	4338	N	GLU	A	614	7.346	31.588	24.010	1.00	24.05		A	N
ANISOU	4338	N	GLU	A	614	2936	2995	3205	4	-24	23	A	N
ATOM	4340	CA	GLU	A	614	8.109	31.722	25.245	1.00	25.20		A	C
ANISOU	4340	CA	GLU	A	614	3167	3172	3234	-3	-38	9	A	C
ATOM	4342	CB	GLU	A	614	8.695	33.131	25.364	1.00	26.82		A	C
ANISOU	4342	CB	GLU	A	614	3352	3350	3487	-24	-40	3	A	C
ATOM	4345	CG	AGLU	A	614	9.853	33.357	24.412	0.40	28.57		A	C
ANISOU	4345	CG	AGLU	A	614	3620	3635	3599	-31	33	20	A	C
ATOM	4346	CG	BGLU	A	614	9.825	33.365	24.378	0.60	29.81		A	C
ANISOU	4346	CG	BGLU	A	614	3758	3786	3781	-38	74	25	A	C
ATOM	4351	CD	AGLU	A	614	10.988	32.383	24.664	0.40	29.71		A	C
ANISOU	4351	CD	AGLU	A	614	3712	3742	3834	11	-21	5	A	C
ATOM	4352	CD	BGLU	A	614	9.338	33.671	22.970	0.60	31.76		A	C
ANISOU	4352	CD	BGLU	A	614	4054	4027	3987	-37	-69	34	A	C
ATOM	4353	OE1	AGLU	A	614	11.424	32.271	25.833	0.40	31.25		A	O
ANISOU	4353	OE1	AGLU	A	614	4016	3978	3876	20	-28	-14	A	O
ATOM	4354	OE1	BGLU	A	614	8.149	34.027	22.796	0.60	33.39		A	O
ANISOU	4354	OE1	BGLU	A	614	4162	4100	4422	-44	41	63	A	O
ATOM	4355	OE2	AGLU	A	614	11.424	31.710	23.704	0.40	30.54		A	O
ANISOU	4355	OE2	AGLU	A	614	3806	3905	3892	-39	67	25	A	O
ATOM	4356	OE2	BGLU	A	614	10.151	33.555	22.027	0.60	34.46		A	O
ANISOU	4356	OE2	BGLU	A	614	4380	4425	4287	-35	63	-39	A	O
ATOM	4357	C	GLU	A	614	7.350	31.332	26.495	1.00	23.98		A	C
ANISOU	4357	C	GLU	A	614	3005	3012	3094	9	-81	-38	A	C
ATOM	4358	O	GLU	A	614	7.910	30.655	27.372	1.00	25.63		A	O
ANISOU	4358	O	GLU	A	614	3169	3232	3338	91	-178	-28	A	O
ATOM	4359	N	ASN	A	615	6.067	31.680	26.555	1.00	21.38		A	N
ANISOU	4359	N	ASN	A	615	2711	2644	2766	-5	-108	-28	A	N
ATOM	4361	CA	ASN	A	615	5.244	31.394	27.711	1.00	20.73		A	C
ANISOU	4361	CA	ASN	A	615	2641	2512	2722	-45	-101	-23	A	C
ATOM	4363	CB	ASN	A	615	4.047	32.334	27.769	1.00	20.77		A	C
ANISOU	4363	CB	ASN	A	615	2674	2496	2719	-10	-75	-36	A	C
ATOM	4366	CG	ASN	A	615	4.418	33.722	28.257	1.00	23.49		A	C
ANISOU	4366	CG	ASN	A	615	3022	2752	3150	-52	-80	-79	A	C
ATOM	4367	OD1	ASN	A	615	5.563	33.961	28.634	1.00	25.36		A	O
ANISOU	4367	OD1	ASN	A	615	3176	2790	3669	-77	-361	-242	A	O
ATOM	4368	ND2	ASN	A	615	3.461	34.642	28.227	1.00	24.27		A	N
ANISOU	4368	ND2	ASN	A	615	2981	3003	3238	-11	-161	-39	A	N
ATOM	4371	C	ASN	A	615	4.731	29.947	27.721	1.00	18.38		A	C
ANISOU	4371	C	ASN	A	615	2369	2213	2400	-17	-42	-39	A	C
ATOM	4372	O	ASN	A	615	4.263	29.460	28.746	1.00	20.15		A	O
ANISOU	4372	O	ASN	A	615	2745	2389	2521	-13	-127	-80	A	O
ATOM	4373	N	ARG	A	616	4.826	29.274	26.583	1.00	16.73		A	N
ANISOU	4373	N	ARG	A	616	2189	1958	2208	-56	-125	40	A	N
ATOM	4375	CA	ARG	A	616	4.343	27.885	26.493	1.00	14.73		A	C
ANISOU	4375	CA	ARG	A	616	1883	1805	1906	-40	-38	-7	A	C
ATOM	4377	CB	ARG	A	616	4.234	27.478	25.018	1.00	14.70		A	C
ANISOU	4377	CB	ARG	A	616	1876	1806	1903	0	-4	-25	A	C
ATOM	4380	CG	ARG	A	616	3.455	26.205	24.759	1.00	13.31		A	C
ANISOU	4380	CG	ARG	A	616	1585	1754	1718	23	-10	72	A	C
ATOM	4383	CD	ARG	A	616	3.426	25.775	23.304	1.00	13.21		A	C
ANISOU	4383	CD	ARG	A	616	1599	1763	1654	-117	-18	-1	A	C
ATOM	4386	NE	ARG	A	616	2.951	26.871	22.459	1.00	13.25		A	N
ANISOU	4386	NE	ARG	A	616	1476	1803	1754	307	126	-61	A	N
ATOM	4388	CZ	ARG	A	616	3.364	27.142	21.212	1.00	13.89		A	C
ANISOU	4388	CZ	ARG	A	616	1829	1753	1695	11	9	-79	A	C
ATOM	4389	NH1	ARG	A	616	4.195	26.320	20.583	1.00	12.76		A	N
ANISOU	4389	NH1	ARG	A	616	1649	1472	1725	134	44	231	A	N

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ATOM	4392	NH2	ARG	A	616	2.934	28.236	20.572	1.00	13.83		A	N
ANISOU	4392	NH2	ARG	A	616	1591	1876	1785	171	89	-29	A	N
ATOM	4395	C	ARG	A	616	5.320	26.980	27.233	1.00	15.28		A	C
ANISOU	4395	C	ARG	A	616	1881	1929	1995	-28	-13	29	A	C
ATOM	4396	O	ARG	A	616	6.536	27.161	27.122	1.00	16.33		A	O
ANISOU	4396	O	ARG	A	616	1991	2058	2152	-82	-90	-30	A	O
ATOM	4397	N	PRO	A	617	4.814	26.019	28.001	1.00	14.80		A	N
ANISOU	4397	N	PRO	A	617	1814	1824	1983	23	-43	4	A	N
ATOM	4398	CA	PRO	A	617	5.706	25.124	28.714	1.00	14.92		A	C
ANISOU	4398	CA	PRO	A	617	1870	1853	1946	-69	-116	-13	A	C
ATOM	4400	CB	PRO	A	617	4.767	24.322	29.614	1.00	15.71		A	C
ANISOU	4400	CB	PRO	A	617	2037	2056	1873	26	-36	65	A	C
ATOM	4403	CG	PRO	A	617	3.448	24.363	28.974	1.00	15.73		A	C
ANISOU	4403	CG	PRO	A	617	1970	1867	2139	33	58	-30	A	C
ATOM	4406	CD	PRO	A	617	3.400	25.684	28.216	1.00	15.43		A	C
ANISOU	4406	CD	PRO	A	617	1914	1889	2059	-7	17	12	A	C
ATOM	4409	C	PRO	A	617	6.438	24.193	27.776	1.00	14.88		A	C
ANISOU	4409	C	PRO	A	617	1799	1937	1914	-13	-45	35	A	C
ATOM	4410	O	PRO	A	617	5.960	23.924	26.679	1.00	14.65		A	O
ANISOU	4410	O	PRO	A	617	1812	1798	1956	-24	-126	-1	A	O
ATOM	4411	N	GLY	A	618	7.618	23.725	28.192	1.00	14.90		A	N
ANISOU	4411	N	GLY	A	618	1816	1926	1919	32	-100	2	A	N
ATOM	4413	CA	GLY	A	618	8.303	22.642	27.492	1.00	14.45		A	C
ANISOU	4413	CA	GLY	A	618	1725	1862	1900	4	-80	50	A	C
ATOM	4416	C	GLY	A	618	7.873	21.304	28.082	1.00	13.99		A	C
ANISOU	4416	C	GLY	A	618	1696	1797	1820	-11	-92	-16	A	C
ATOM	4417	O	GLY	A	618	7.103	21.226	29.060	1.00	14.71		A	O
ANISOU	4417	O	GLY	A	618	1848	1818	1922	35	-95	20	A	O
ATOM	4418	N	PHE	A	619	8.345	20.235	27.477	1.00	14.29		A	N
ANISOU	4418	N	PHE	A	619	1700	1837	1890	51	-37	69	A	N
ATOM	4420	CA	PHE	A	619	7.903	18.927	27.929	1.00	14.02		A	C
ANISOU	4420	CA	PHE	A	619	1762	1790	1775	-5	-60	70	A	C
ATOM	4422	CB	PHE	A	619	8.301	17.835	26.959	1.00	14.69		A	C
ANISOU	4422	CB	PHE	A	619	1855	1980	1746	79	-42	90	A	C
ATOM	4425	CG	PHE	A	619	7.406	17.737	25.784	1.00	13.02		A	C
ANISOU	4425	CG	PHE	A	619	1550	1678	1719	73	-22	28	A	C
ATOM	4426	CD1	PHE	A	619	6.141	17.238	25.919	1.00	12.41		A	C
ANISOU	4426	CD1	PHE	A	619	1601	1508	1604	65	-64	154	A	C
ATOM	4428	CE1	PHE	A	619	5.307	17.145	24.836	1.00	13.75		A	C
ANISOU	4428	CE1	PHE	A	619	1622	1843	1757	-8	-73	-16	A	C
ATOM	4430	CZ	PHE	A	619	5.722	17.553	23.610	1.00	12.93		A	C
ANISOU	4430	CZ	PHE	A	619	1495	1649	1769	24	-61	-3	A	C
ATOM	4432	CE2	PHE	A	619	6.980	18.052	23.452	1.00	12.36		A	C
ANISOU	4432	CE2	PHE	A	619	1355	1718	1624	163	15	124	A	C
ATOM	4434	CD2	PHE	A	619	7.830	18.146	24.535	1.00	13.25		A	C
ANISOU	4434	CD2	PHE	A	619	1679	1653	1701	14	-37	49	A	C
ATOM	4436	C	PHE	A	619	8.355	18.559	29.343	1.00	15.14		A	C
ANISOU	4436	C	PHE	A	619	1925	1986	1841	-56	-107	58	A	C
ATOM	4437	O	PHE	A	619	7.687	17.777	30.015	1.00	15.59		A	O
ANISOU	4437	O	PHE	A	619	1951	2133	1839	28	-155	141	A	O
ATOM	4438	N	ALA	A	620	9.485	19.076	29.798	1.00	15.95		A	N
ANISOU	4438	N	ALA	A	620	1989	2060	2011	-2	-125	122	A	N
ATOM	4440	CA	ALA	A	620	9.831	18.792	31.182	1.00	17.25		A	C
ANISOU	4440	CA	ALA	A	620	2235	2190	2129	-60	-122	79	A	C
ATOM	4442	CB	ALA	A	620	11.205	19.386	31.532	1.00	18.01		A	C
ANISOU	4442	CB	ALA	A	620	2297	2388	2157	-62	-120	70	A	C
ATOM	4446	C	ALA	A	620	8.715	19.242	32.138	1.00	17.40		A	C
ANISOU	4446	C	ALA	A	620	2299	2166	2145	-89	-164	8	A	C
ATOM	4447	O	ALA	A	620	8.258	18.474	33.016	1.00	18.72		A	O
ANISOU	4447	O	ALA	A	620	2581	2436	2093	-50	-261	66	A	O
ATOM	4448	N	ALA	A	621	8.203	20.464	31.949	1.00	17.11		A	N
ANISOU	4448	N	ALA	A	621	2172	2129	2198	-6	-135	56	A	N

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ATOM	4450	CA	ALA	A	621	7.139	20.980	32.804	1.00	17.79		A	C
ANISOU	4450	CA	ALA	A	621	2304	2260	2193	-11	-96	41	A	C
ATOM	4452	CB	ALA	A	621	6.888	22.445	32.512	1.00	18.61		A	C
ANISOU	4452	CB	ALA	A	621	2424	2352	2293	-49	-121	7	A	C
ATOM	4456	C	ALA	A	621	5.840	20.196	32.620	1.00	16.92		A	C
ANISOU	4456	C	ALA	A	621	2222	2098	2105	-1	-45	7	A	C
ATOM	4457	O	ALA	A	621	5.127	19.899	33.571	1.00	18.02		A	O
ANISOU	4457	O	ALA	A	621	2525	2194	2125	58	-93	51	A	O
ATOM	4458	N	VAL	A	622	5.495	19.914	31.368	1.00	15.98		A	N
ANISOU	4458	N	VAL	A	622	2106	2017	1945	22	-17	-3	A	N
ATOM	4460	CA	VAL	A	622	4.281	19.174	31.072	1.00	15.39		A	C
ANISOU	4460	CA	VAL	A	622	2025	1948	1873	40	-15	12	A	C
ATOM	4462	CB	VAL	A	622	4.083	19.080	29.544	1.00	15.52		A	C
ANISOU	4462	CB	VAL	A	622	2023	1946	1926	46	-108	26	A	C
ATOM	4464	CG1	VAL	A	622	2.968	18.097	29.178	1.00	14.94		A	C
ANISOU	4464	CG1	VAL	A	622	1986	1813	1876	-45	-30	199	A	C
ATOM	4468	CG2	VAL	A	622	3.796	20.462	28.980	1.00	15.95		A	C
ANISOU	4468	CG2	VAL	A	622	1992	1946	2123	-116	-160	42	A	C
ATOM	4472	C	VAL	A	622	4.315	17.777	31.687	1.00	15.76		A	C
ANISOU	4472	C	VAL	A	622	2031	2040	1915	57	-56	37	A	C
ATOM	4473	O	VAL	A	622	3.343	17.342	32.291	1.00	16.84		A	O
ANISOU	4473	O	VAL	A	622	2111	2256	2030	215	-6	154	A	O
ATOM	4474	N	GLU	A	623	5.426	17.074	31.501	1.00	15.32		A	N
ANISOU	4474	N	GLU	A	623	1910	2008	1903	22	-67	-1	A	N
ATOM	4476	CA	GLU	A	623	5.547	15.740	32.034	1.00	16.28		A	C
ANISOU	4476	CA	GLU	A	623	2100	2095	1987	26	-56	-1	A	C
ATOM	4478	CB	GLU	A	623	6.864	15.073	31.608	1.00	15.94		A	C
ANISOU	4478	CB	GLU	A	623	1966	2084	2006	33	-183	47	A	C
ATOM	4481	CG	GLU	A	623	6.976	13.605	32.028	1.00	18.08		A	C
ANISOU	4481	CG	GLU	A	623	2367	2225	2276	-11	-68	22	A	C
ATOM	4484	CD	GLU	A	623	7.426	13.418	33.480	1.00	20.16		A	C
ANISOU	4484	CD	GLU	A	623	2610	2625	2422	-83	-131	92	A	C
ATOM	4485	OE1	GLU	A	623	8.209	14.263	33.968	1.00	21.23		A	O
ANISOU	4485	OE1	GLU	A	623	2927	2434	2704	-46	-261	135	A	O
ATOM	4486	OE2	GLU	A	623	7.036	12.406	34.115	1.00	20.34		A	O
ANISOU	4486	OE2	GLU	A	623	2665	2534	2529	-62	-240	147	A	O
ATOM	4487	C	GLU	A	623	5.403	15.762	33.545	1.00	16.50		A	C
ANISOU	4487	C	GLU	A	623	2108	2145	2017	9	-59	70	A	C
ATOM	4488	O	GLU	A	623	4.787	14.876	34.097	1.00	17.07		A	O
ANISOU	4488	O	GLU	A	623	2120	2278	2088	-2	-143	152	A	O
ATOM	4489	N	LEU	A	624	5.999	16.760	34.204	1.00	16.82		A	N
ANISOU	4489	N	LEU	A	624	2278	2155	1956	0	-85	28	A	N
ATOM	4491	CA	LEU	A	624	5.932	16.837	35.676	1.00	18.65		A	C
ANISOU	4491	CA	LEU	A	624	2509	2364	2211	-2	-48	8	A	C
ATOM	4493	CB	LEU	A	624	6.813	17.961	36.202	1.00	19.86		A	C
ANISOU	4493	CB	LEU	A	624	2644	2547	2355	-24	-72	0	A	C
ATOM	4496	CG	LEU	A	624	6.932	18.039	37.728	1.00	23.05		A	C
ANISOU	4496	CG	LEU	A	624	3058	3058	2643	-64	-7	-72	A	C
ATOM	4498	CD1	LEU	A	624	7.374	16.744	38.281	1.00	24.62		A	C
ANISOU	4498	CD1	LEU	A	624	3261	3194	2898	-74	-128	-63	A	C
ATOM	4502	CD2	LEU	A	624	7.912	19.123	38.118	1.00	25.62		A	C
ANISOU	4502	CD2	LEU	A	624	3327	3293	3112	-133	-89	-57	A	C
ATOM	4506	C	LEU	A	624	4.518	17.042	36.134	1.00	19.24		A	C
ANISOU	4506	C	LEU	A	624	2602	2431	2274	-28	-52	-41	A	C
ATOM	4507	O	LEU	A	624	4.041	16.377	37.061	1.00	19.93		A	O
ANISOU	4507	O	LEU	A	624	2951	2414	2207	-80	-145	-50	A	O
ATOM	4508	N	ARG	A	625	3.809	17.956	35.487	1.00	20.61		A	N
ANISOU	4508	N	ARG	A	625	2788	2598	2443	35	-39	47	A	N
ATOM	4510	CA	ARG	A	625	2.443	18.216	35.918	1.00	22.08		A	C
ANISOU	4510	CA	ARG	A	625	2877	2842	2670	59	2	36	A	C
ATOM	4512	CB	ARG	A	625	1.824	19.401	35.157	1.00	24.05		A	C
ANISOU	4512	CB	ARG	A	625	3153	3042	2942	91	-56	97	A	C



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ATOM	4515	CG	AARG	A	625	0.627	20.008	35.859	0.50	26.09		A	C
ANISOU	4515	CG	AARG	A	625	3289	3353	3271	21	38	-3	A	C
ATOM	4516	CG	BARG	A	625	0.658	20.071	35.903	0.50	26.60		A	C
ANISOU	4516	CG	BARG	A	625	3358	3415	3331	19	53	-23	A	C
ATOM	4521	CD	AARG	A	625	0.098	21.275	35.209	0.50	29.42		A	C
ANISOU	4521	CD	AARG	A	625	3821	3664	3693	66	-20	60	A	C
ATOM	4522	CD	BARG	A	625	0.010	21.269	35.179	0.50	30.50		A	C
ANISOU	4522	CD	BARG	A	625	3926	3811	3852	22	-40	115	A	C
ATOM	4527	NE	AARG	A	625	1.168	22.232	34.958	0.50	31.57		A	N
ANISOU	4527	NE	AARG	A	625	3947	4002	4044	-32	-22	19	A	N
ATOM	4528	NE	BARG	A	625	-0.565	22.250	36.104	0.50	33.28		A	N
ANISOU	4528	NE	BARG	A	625	4271	4180	4190	-3	45	-41	A	N
ATOM	4531	CZ	AARG	A	625	1.225	23.458	35.462	0.50	33.50		A	C
ANISOU	4531	CZ	AARG	A	625	4299	4176	4253	3	-11	-32	A	C
ATOM	4532	CZ	BARG	A	625	-1.670	22.961	35.879	0.50	35.81		A	C
ANISOU	4532	CZ	BARG	A	625	4499	4528	4577	21	-36	27	A	C
ATOM	4533	NH1AARG	A	625	0.261	23.909	36.250	0.50	34.24			A	N
ANISOU	4533	NH1AARG	A	625	4343	4312	4353	20	27	-10	A	N	
ATOM	4534	NH1BARG	A	625	-2.353	22.807	34.757	0.50	36.74			A	N
ANISOU	4534	NH1BARG	A	625	4676	4681	4601	9	-52	19	A	N	
ATOM	4539	NH2AARG	A	625	2.257	24.237	35.171	0.50	34.40			A	N
ANISOU	4539	NH2AARG	A	625	4394	4345	4328	-85	-24	-20	A	N	
ATOM	4540	NH2BARG	A	625	-2.112	23.824	36.791	0.50	37.36			A	N
ANISOU	4540	NH2BARG	A	625	4738	4693	4764	30	18	-16	A	N	
ATOM	4545	C	ARG	A	625	1.602	16.979	35.711	1.00	21.43		A	C
ANISOU	4545	C	ARG	A	625	2793	2805	2542	92	-15	41	A	C
ATOM	4546	O	ARG	A	625	0.777	16.623	36.551	1.00	22.03		A	O
ANISOU	4546	O	ARG	A	625	3043	2988	2336	152	103	-15	A	O
ATOM	4547	N	LEU	A	626	1.764	16.332	34.555	1.00	19.85		A	N
ANISOU	4547	N	LEU	A	626	2648	2638	2256	182	80	60	A	N
ATOM	4549	CA	LEU	A	626	1.026	15.134	34.256	1.00	20.60		A	C
ANISOU	4549	CA	LEU	A	626	2645	2747	2432	65	-3	15	A	C
ATOM	4551	CB	LEU	A	626	1.345	14.575	32.879	1.00	21.94		A	C
ANISOU	4551	CB	LEU	A	626	2828	2918	2589	132	116	53	A	C
ATOM	4554	CG	LEU	A	626	0.247	14.676	31.872	1.00	23.72		A	C
ANISOU	4554	CG	LEU	A	626	3001	3150	2859	13	28	-97	A	C
ATOM	4556	CD1	LEU	A	626	0.766	14.218	30.530	1.00	22.12		A	C
ANISOU	4556	CD1	LEU	A	626	2695	2990	2718	141	26	-83	A	C
ATOM	4560	CD2	LEU	A	626	-1.077	14.015	32.234	1.00	23.81		A	C
ANISOU	4560	CD2	LEU	A	626	3012	3093	2941	34	27	-3	A	C
ATOM	4564	C	LEU	A	626	1.307	14.012	35.218	1.00	20.36		A	C
ANISOU	4564	C	LEU	A	626	2674	2622	2438	27	-20	12	A	C
ATOM	4565	O	LEU	A	626	0.396	13.317	35.615	1.00	21.31		A	O
ANISOU	4565	O	LEU	A	626	2713	3007	2376	-9	-113	80	A	O
ATOM	4566	N	ARG	A	627	2.587	13.810	35.518	1.00	19.76		A	N
ANISOU	4566	N	ARG	A	627	2647	2495	2366	4	-57	46	A	N
ATOM	4568	CA	ARG	A	627	3.041	12.760	36.438	1.00	20.40		A	C
ANISOU	4568	CA	ARG	A	627	2686	2537	2526	20	-27	42	A	C
ATOM	4570	CB	ARG	A	627	4.551	12.879	36.578	1.00	20.22		A	C
ANISOU	4570	CB	ARG	A	627	2655	2521	2507	20	-24	83	A	C
ATOM	4573	CG	ARG	A	627	5.238	11.769	37.334	1.00	21.05		A	C
ANISOU	4573	CG	ARG	A	627	2815	2611	2572	46	18	50	A	C
ATOM	4576	CD	ARG	A	627	6.512	12.185	37.964	1.00	23.18		A	C
ANISOU	4576	CD	ARG	A	627	2883	2999	2925	98	-23	11	A	C
ATOM	4579	NE	ARG	A	627	7.463	12.755	37.029	1.00	26.02		A	N
ANISOU	4579	NE	ARG	A	627	3289	3429	3165	-76	-21	93	A	N
ATOM	4581	CZ	ARG	A	627	8.603	13.358	37.394	1.00	29.21		A	C
ANISOU	4581	CZ	ARG	A	627	3625	3826	3644	-135	-74	-30	A	C
ATOM	4582	NH1	ARG	A	627	8.927	13.430	38.687	1.00	30.80		A	N
ANISOU	4582	NH1	ARG	A	627	3961	4086	3654	-80	-84	-1	A	N
ATOM	4585	NH2	ARG	A	627	9.423	13.875	36.479	1.00	29.20		A	N
ANISOU	4585	NH2	ARG	A	627	3710	3819	3564	-122	-95	17	A	N

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ATOM	4588	C	ARG	A	627	2.390	12.931	37.799	1.00	21.10		A	C
ANISOU	4588	C	ARG	A	627	2734	2683	2598	-33	-50	58	A	C
ATOM	4589	O	ARG	A	627	1.838	11.982	38.365	1.00	20.69		A	O
ANISOU	4589	O	ARG	A	627	2724	2687	2447	-24	-136	171	A	O
ATOM	4590	N	ASN	A	628	2.446	14.155	38.318	1.00	21.67		A	N
ANISOU	4590	N	ASN	A	628	2788	2804	2641	31	-11	3	A	N
ATOM	4592	CA	ASN	A	628	1.910	14.414	39.655	1.00	22.14		A	C
ANISOU	4592	CA	ASN	A	628	2899	2902	2611	12	-15	36	A	C
ATOM	4594	CB	ASN	A	628	2.286	15.808	40.138	1.00	23.42		A	C
ANISOU	4594	CB	ASN	A	628	3077	3065	2754	2	41	34	A	C
ATOM	4597	CG	ASN	A	628	3.782	15.945	40.438	1.00	23.76		A	C
ANISOU	4597	CG	ASN	A	628	3186	3195	2647	5	-20	-41	A	C
ATOM	4598	OD1	ASN	A	628	4.473	14.967	40.732	1.00	25.16		A	O
ANISOU	4598	OD1	ASN	A	628	3210	3730	2617	106	-181	-46	A	O
ATOM	4599	ND2	ASN	A	628	4.287	17.164	40.314	1.00	26.41		A	N
ANISOU	4599	ND2	ASN	A	628	3566	3502	2965	-192	27	-134	A	N
ATOM	4602	C	ASN	A	628	0.416	14.164	39.698	1.00	22.62		A	C
ANISOU	4602	C	ASN	A	628	2961	2970	2662	36	-9	39	A	C
ATOM	4603	O	ASN	A	628	-0.098	13.588	40.653	1.00	22.98		A	O
ANISOU	4603	O	ASN	A	628	3074	3018	2637	-10	-89	152	A	O
ATOM	4604	N	TYR	A	629	-0.302	14.571	38.655	1.00	21.53		A	N
ANISOU	4604	N	TYR	A	629	2885	2842	2452	41	-10	60	A	N
ATOM	4606	CA	TYR	A	629	-1.723	14.334	38.600	1.00	21.60		A	C
ANISOU	4606	CA	TYR	A	629	2882	2798	2527	39	4	38	A	C
ATOM	4608	CB	TYR	A	629	-2.344	15.133	37.453	1.00	21.68		A	C
ANISOU	4608	CB	TYR	A	629	2976	2755	2504	27	59	32	A	C
ATOM	4611	CG	TYR	A	629	-3.795	14.903	37.317	1.00	22.86		A	C
ANISOU	4611	CG	TYR	A	629	3128	2800	2757	59	-62	186	A	C
ATOM	4612	CD1	TYR	A	629	-4.684	15.284	38.309	1.00	24.82		A	C
ANISOU	4612	CD1	TYR	A	629	3182	3090	3157	64	-16	51	A	C
ATOM	4614	CE1	TYR	A	629	-6.041	15.029	38.170	1.00	27.68		A	C
ANISOU	4614	CE1	TYR	A	629	3439	3551	3524	-23	-14	124	A	C
ATOM	4616	CZ	TYR	A	629	-6.465	14.383	37.019	1.00	27.78		A	C
ANISOU	4616	CZ	TYR	A	629	3570	3401	3581	36	10	43	A	C
ATOM	4617	OH	TYR	A	629	-7.762	14.074	36.751	1.00	32.66		A	O
ANISOU	4617	OH	TYR	A	629	3876	4134	4399	-26	-130	55	A	O
ATOM	4619	CE2	TYR	A	629	-5.589	13.999	36.071	1.00	26.91		A	C
ANISOU	4619	CE2	TYR	A	629	3460	3398	3364	-43	-40	136	A	C
ATOM	4621	CD2	TYR	A	629	-4.284	14.260	36.210	1.00	25.44		A	C
ANISOU	4621	CD2	TYR	A	629	3337	3185	3142	-1	-87	18	A	C
ATOM	4623	C	TYR	A	629	-2.036	12.838	38.479	1.00	21.66		A	C
ANISOU	4623	C	TYR	A	629	2793	2832	2604	35	-29	61	A	C
ATOM	4624	O	TYR	A	629	-2.937	12.329	39.137	1.00	22.50		A	O
ANISOU	4624	O	TYR	A	629	3006	2960	2581	25	8	66	A	O
ATOM	4625	N	TYR	A	630	-1.273	12.128	37.661	1.00	21.42		A	N
ANISOU	4625	N	TYR	A	630	2876	2787	2475	-11	-14	55	A	N
ATOM	4627	CA	TYR	A	630	-1.485	10.712	37.474	1.00	21.75		A	C
ANISOU	4627	CA	TYR	A	630	2825	2821	2617	14	-11	66	A	C
ATOM	4629	CB	TYR	A	630	-0.498	10.153	36.450	1.00	22.03		A	C
ANISOU	4629	CB	TYR	A	630	2899	2770	2701	27	-29	59	A	C
ATOM	4632	CG	TYR	A	630	-0.606	8.675	36.284	1.00	21.06		A	C
ANISOU	4632	CG	TYR	A	630	2762	2768	2470	-47	-14	0	A	C
ATOM	4633	CD1	TYR	A	630	-1.829	8.062	36.017	1.00	20.63		A	C
ANISOU	4633	CD1	TYR	A	630	2610	2733	2493	7	77	76	A	C
ATOM	4635	CE1	TYR	A	630	-1.913	6.702	35.879	1.00	21.36		A	C
ANISOU	4635	CE1	TYR	A	630	2705	2799	2611	-37	-6	-28	A	C
ATOM	4637	CZ	TYR	A	630	-0.785	5.932	36.041	1.00	22.59		A	C
ANISOU	4637	CZ	TYR	A	630	2828	2918	2837	2	-22	-21	A	C
ATOM	4638	OH	TYR	A	630	-0.851	4.571	35.949	1.00	25.11		A	O
ANISOU	4638	OH	TYR	A	630	3479	2999	3063	112	-25	76	A	O
ATOM	4640	CE2	TYR	A	630	0.430	6.520	36.313	1.00	23.76		A	C
ANISOU	4640	CE2	TYR	A	630	3066	2978	2983	-20	-64	7	A	C

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ATOM	4642	CD2	TYR	A	630	0.508	7.878	36.438	1.00	22.13		A	C
ANISOU	4642	CD2	TYR	A	630	2836	2855	2716	-48	-28	43	A	C
ATOM	4644	C	TYR	A	630	-1.316	9.996	38.813	1.00	22.13		A	C
ANISOU	4644	C	TYR	A	630	2909	2820	2676	11	14	86	A	C
ATOM	4645	O	TYR	A	630	-2.164	9.199	39.201	1.00	22.80		A	O
ANISOU	4645	O	TYR	A	630	3046	2990	2624	29	10	35	A	O
ATOM	4646	N	TYR	A	631	-0.209	10.263	39.488	1.00	23.30		A	N
ANISOU	4646	N	TYR	A	631	3093	3014	2744	-17	8	80	A	N
ATOM	4648	CA	TYR	A	631	0.050	9.603	40.771	1.00	24.46		A	C
ANISOU	4648	CA	TYR	A	631	3227	3060	3004	31	-20	116	A	C
ATOM	4650	CB	TYR	A	631	1.383	10.036	41.386	1.00	24.29		A	C
ANISOU	4650	CB	TYR	A	631	3199	3112	2916	25	-4	150	A	C
ATOM	4653	CG	TYR	A	631	2.593	9.643	40.609	1.00	24.75		A	C
ANISOU	4653	CG	TYR	A	631	3276	3122	3004	68	-87	121	A	C
ATOM	4654	CD1	TYR	A	631	2.524	8.700	39.599	1.00	26.39		A	C
ANISOU	4654	CD1	TYR	A	631	3472	3245	3308	93	-35	49	A	C
ATOM	4656	CE1	TYR	A	631	3.637	8.371	38.876	1.00	26.33		A	C
ANISOU	4656	CE1	TYR	A	631	3413	3291	3300	45	20	109	A	C
ATOM	4658	CZ	TYR	A	631	4.826	8.983	39.171	1.00	26.97		A	C
ANISOU	4658	CZ	TYR	A	631	3562	3286	3398	35	-88	80	A	C
ATOM	4659	OH	TYR	A	631	5.962	8.694	38.472	1.00	30.70		A	O
ANISOU	4659	OH	TYR	A	631	4003	3776	3885	184	127	96	A	O
ATOM	4661	CE2	TYR	A	631	4.912	9.914	40.164	1.00	25.54		A	C
ANISOU	4661	CE2	TYR	A	631	3319	3182	3202	95	18	106	A	C
ATOM	4663	CD2	TYR	A	631	3.808	10.246	40.862	1.00	24.63		A	C
ANISOU	4663	CD2	TYR	A	631	3218	3181	2958	46	-6	190	A	C
ATOM	4665	C	TYR	A	631	-1.085	9.896	41.736	1.00	25.94		A	C
ANISOU	4665	C	TYR	A	631	3396	3285	3173	35	52	66	A	C
ATOM	4666	O	TYR	A	631	-1.440	9.031	42.539	1.00	26.98		A	O
ANISOU	4666	O	TYR	A	631	3627	3386	3237	122	79	141	A	O
ATOM	4667	N	ASP	A	632	-1.671	11.095	41.670	1.00	27.38		A	N
ANISOU	4667	N	ASP	A	632	3571	3449	3380	27	-4	73	A	N
ATOM	4669	CA	ASP	A	632	-2.781	11.440	42.561	1.00	28.96		A	C
ANISOU	4669	CA	ASP	A	632	3731	3666	3607	9	21	18	A	C
ATOM	4671	CB	ASP	A	632	-3.106	12.917	42.467	1.00	30.21		A	C
ANISOU	4671	CB	ASP	A	632	3873	3791	3811	54	-10	55	A	C
ATOM	4674	CG	ASP	A	632	-3.687	13.485	43.747	1.00	33.26		A	C
ANISOU	4674	CG	ASP	A	632	4295	4236	4105	41	51	-53	A	C
ATOM	4675	OD1	ASP	A	632	-3.614	12.839	44.827	1.00	35.88		A	O
ANISOU	4675	OD1	ASP	A	632	4712	4623	4297	9	75	84	A	O
ATOM	4676	OD2	ASP	A	632	-4.239	14.606	43.744	1.00	37.23		A	O
ANISOU	4676	OD2	ASP	A	632	4829	4491	4824	136	-38	-51	A	O
ATOM	4677	C	ASP	A	632	-4.026	10.648	42.243	1.00	29.27		A	C
ANISOU	4677	C	ASP	A	632	3747	3694	3678	22	15	25	A	C
ATOM	4678	O	ASP	A	632	-4.702	10.154	43.153	1.00	29.89		A	O
ANISOU	4678	O	ASP	A	632	3907	3786	3663	55	77	45	A	O
ATOM	4679	N	VAL	A	633	-4.322	10.511	40.953	1.00	29.07		A	N
ANISOU	4679	N	VAL	A	633	3764	3677	3604	0	28	59	A	N
ATOM	4681	CA	VAL	A	633	-5.487	9.752	40.507	1.00	29.63		A	C
ANISOU	4681	CA	VAL	A	633	3776	3763	3718	8	2	34	A	C
ATOM	4683	CB	VAL	A	633	-5.719	9.922	38.990	1.00	29.93		A	C
ANISOU	4683	CB	VAL	A	633	3825	3790	3756	-14	15	41	A	C
ATOM	4685	CG1	VAL	A	633	-6.779	8.953	38.476	1.00	30.76		A	C
ANISOU	4685	CG1	VAL	A	633	3848	3948	3889	2	2	57	A	C
ATOM	4689	CG2	VAL	A	633	-6.094	11.364	38.678	1.00	29.72		A	C
ANISOU	4689	CG2	VAL	A	633	3781	3790	3720	60	-2	-36	A	C
ATOM	4693	C	VAL	A	633	-5.332	8.266	40.833	1.00	29.99		A	C
ANISOU	4693	C	VAL	A	633	3826	3805	3761	-8	-4	72	A	C
ATOM	4694	O	VAL	A	633	-6.298	7.591	41.170	1.00	30.51		A	O
ANISOU	4694	O	VAL	A	633	3863	3826	3904	16	-26	110	A	O
ATOM	4695	N	VAL	A	634	-4.119	7.760	40.727	1.00	29.96		A	N
ANISOU	4695	N	VAL	A	634	3811	3836	3733	-12	32	59	A	N

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ATOM	4697	CA	VAL A 634	-3.854	6.367	41.037	1.00	31.14		A	C
ANISOU	4697	CA	VAL A 634	3996	3949	3884	-11	11	35	A	C
ATOM	4699	CB	VAL A 634	-2.433	5.980	40.655	1.00	31.08		A	C
ANISOU	4699	CB	VAL A 634	3985	3942	3882	14	0	37	A	C
ATOM	4701	CG1	VAL A 634	-2.074	4.628	41.244	1.00	31.82		A	C
ANISOU	4701	CG1	VAL A 634	4172	3959	3955	14	-11	37	A	C
ATOM	4705	CG2	VAL A 634	-2.288	5.954	39.134	1.00	30.75		A	C
ANISOU	4705	CG2	VAL A 634	3962	3859	3860	-9	8	8	A	C
ATOM	4709	C	VAL A 634	-4.080	6.116	42.531	1.00	32.40		A	C
ANISOU	4709	C	VAL A 634	4188	4126	3996	-30	15	50	A	C
ATOM	4710	O	VAL A 634	-4.491	5.023	42.924	1.00	33.53		A	O
ANISOU	4710	O	VAL A 634	4321	4294	4122	-108	10	104	A	O
ATOM	4711	N	ASN A 635	-3.749	7.111	43.344	1.00	33.27		A	N
ANISOU	4711	N	ASN A 635	4286	4250	4106	-13	33	20	A	N
ATOM	4713	CA	ASN A 635	-4.043	7.080	44.777	1.00	34.04		A	C
ANISOU	4713	CA	ASN A 635	4353	4381	4198	2	14	28	A	C
ATOM	4715	CB	ASN A 635	-3.333	8.214	45.494	1.00	33.81		A	C
ANISOU	4715	CB	ASN A 635	4312	4323	4210	27	8	7	A	C
ATOM	4718	CG	ASN A 635	-3.296	8.013	47.009	1.00	34.33		A	C
ANISOU	4718	CG	ASN A 635	4421	4353	4269	8	76	23	A	C
ATOM	4719	OD1	ASN A 635	-3.447	8.961	47.776	1.00	35.61		A	O
ANISOU	4719	OD1	ASN A 635	4584	4616	4327	-15	101	-53	A	O
ATOM	4720	ND2	ASN A 635	-3.093	6.770	47.437	1.00	33.88		A	N
ANISOU	4720	ND2	ASN A 635	4317	4423	4130	69	82	88	A	N
ATOM	4723	C	ASN A 635	-5.518	7.309	45.017	1.00	34.58		A	C
ANISOU	4723	C	ASN A 635	4388	4492	4258	4	16	20	A	C
ATOM	4724	O	ASN A 635	-6.297	7.622	44.129	1.00	35.21		A	O
ANISOU	4724	O	ASN A 635	4527	4553	4296	-8	10	55	A	O
ATOM	4725	OXT	ASN A 635	-6.017	7.265	46.144	1.00	36.83		A	O
ANISOU	4725	OXT	ASN A 635	4680	4793	4519	15	77	70	A	O
ATOM	4726	O5	STU B 1	3.339	-1.531	15.205	1.00	18.13		B	O
ANISOU	4726	O5	STU B 1	2459	2351	2076	38	85	119	B	O
ATOM	4727	C8	STU B 1	3.903	-0.614	14.513	1.00	17.58		B	C
ANISOU	4727	C8	STU B 1	2404	2166	2107	172	115	92	B	C
ATOM	4728	N1	STU B 1	5.176	-0.232	14.561	1.00	17.13		B	N
ANISOU	4728	N1	STU B 1	2435	2028	2043	236	119	-27	B	N
ATOM	4729	C7	STU B 1	3.102	0.191	13.575	1.00	16.94		B	C
ANISOU	4729	C7	STU B 1	2329	2051	2055	137	55	-47	B	C
ATOM	4730	C6	STU B 1	1.689	0.245	13.233	1.00	16.77		B	C
ANISOU	4730	C6	STU B 1	2477	1756	2138	41	-91	-130	B	C
ATOM	4731	C5	STU B 1	0.516	-0.495	13.659	1.00	17.66		B	C
ANISOU	4731	C5	STU B 1	2442	2147	2119	9	41	-194	B	C
ATOM	4732	C20	STU B 1	-0.601	0.081	12.896	1.00	18.68		B	C
ANISOU	4732	C20	STU B 1	2616	2207	2276	48	-49	-72	B	C
ATOM	4733	C1	STU B 1	-1.890	-0.370	13.042	1.00	19.40		B	C
ANISOU	4733	C1	STU B 1	2591	2258	2521	71	-21	-1	B	C
ATOM	4735	C2	STU B 1	-2.080	-1.413	13.944	1.00	19.98		B	C
ANISOU	4735	C2	STU B 1	2513	2441	2639	-114	-45	59	B	C
ATOM	4737	C3	STU B 1	-1.011	-1.957	14.675	1.00	18.60		B	C
ANISOU	4737	C3	STU B 1	2374	2198	2495	-21	-54	19	B	C
ATOM	4739	C4	STU B 1	0.325	-1.522	14.553	1.00	17.56		B	C
ANISOU	4739	C4	STU B 1	2413	2059	2199	-100	-17	-4	B	C
ATOM	4741	N3	STU B 1	-0.126	1.092	12.069	1.00	18.40		B	N
ANISOU	4741	N3	STU B 1	2402	2135	2451	-144	-80	-68	B	N
ATOM	4742	C19	STU B 1	1.234	1.205	12.238	1.00	17.83		B	C
ANISOU	4742	C19	STU B 1	2487	2072	2214	84	-91	-26	B	C
ATOM	4743	C25	STU B 1	-0.931	1.866	11.154	1.00	20.53		B	C
ANISOU	4743	C25	STU B 1	2643	2515	2641	-20	-22	85	B	C
ATOM	4745	O4	STU B 1	-0.062	2.241	10.101	1.00	19.66		B	O
ANISOU	4745	O4	STU B 1	2818	2219	2431	69	-100	19	B	O
ATOM	4746	C10	STU B 1	4.090	1.067	13.029	1.00	15.75		B	C
ANISOU	4746	C10	STU B 1	2268	1775	1940	204	80	-229	B	C

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ATOM	4747	C9	STU	B	1	5.351	0.767	13.620	1.00	17.11		B	C
ANISOU	4747	C9	STU	B	1	2215	2042	2241	130	23	-5	B	C
ATOM	4749	C11	STU	B	1	3.627	2.041	12.021	1.00	16.38		B	C
ANISOU	4749	C11	STU	B	1	2313	2040	1868	108	68	-151	B	C
ATOM	4750	C12	STU	B	1	4.274	3.096	11.268	1.00	17.90		B	C
ANISOU	4750	C12	STU	B	1	2522	2041	2236	12	83	-120	B	C
ATOM	4751	C13	STU	B	1	5.596	3.473	11.255	1.00	18.63		B	C
ANISOU	4751	C13	STU	B	1	2429	2354	2294	87	111	-48	B	C
ATOM	4753	C14	STU	B	1	5.943	4.537	10.416	1.00	19.48		B	C
ANISOU	4753	C14	STU	B	1	2727	2410	2263	123	56	-101	B	C
ATOM	4755	C15	STU	B	1	4.982	5.162	9.622	1.00	19.25		B	C
ANISOU	4755	C15	STU	B	1	2526	2472	2316	20	25	-115	B	C
ATOM	4757	C17	STU	B	1	3.233	3.743	10.444	1.00	18.34		B	C
ANISOU	4757	C17	STU	B	1	2485	2229	2253	-14	6	-30	B	C
ATOM	4758	C16	STU	B	1	3.649	4.790	9.618	1.00	19.67		B	C
ANISOU	4758	C16	STU	B	1	2572	2526	2374	58	93	58	B	C
ATOM	4760	C18	STU	B	1	2.216	2.102	11.647	1.00	17.21		B	C
ANISOU	4760	C18	STU	B	1	2364	2082	2092	46	-51	-56	B	C
ATOM	4761	N2	STU	B	1	2.072	3.094	10.736	1.00	19.21		B	N
ANISOU	4761	N2	STU	B	1	2762	2179	2357	-30	-27	131	B	N
ATOM	4762	C21	STU	B	1	0.714	3.432	10.237	1.00	19.85		B	C
ANISOU	4762	C21	STU	B	1	2599	2507	2434	-136	34	36	B	C
ATOM	4763	C26	STU	B	1	0.718	4.018	8.824	1.00	21.00		B	C
ANISOU	4763	C26	STU	B	1	2789	2576	2611	31	-10	64	B	C
ATOM	4767	C22	STU	B	1	0.111	4.444	11.245	1.00	20.02		B	C
ANISOU	4767	C22	STU	B	1	2677	2401	2528	13	-81	99	B	C
ATOM	4769	O6	STU	B	1	0.538	4.256	12.604	1.00	19.96		B	O
ANISOU	4769	O6	STU	B	1	2739	2391	2451	-2	-119	-55	B	O
ATOM	4770	C27	STU	B	1	1.577	5.139	13.065	1.00	19.81		B	C
ANISOU	4770	C27	STU	B	1	2539	2355	2631	-42	36	97	B	C
ATOM	4774	C23	STU	B	1	-1.398	4.320	11.340	1.00	20.74		B	C
ANISOU	4774	C23	STU	B	1	2724	2618	2538	-61	-45	66	B	C
ATOM	4776	C24	STU	B	1	-1.671	2.949	11.925	1.00	20.25		B	C
ANISOU	4776	C24	STU	B	1	2619	2468	2607	33	-163	15	B	C
ATOM	4779	N4	STU	B	1	-2.050	5.355	12.163	1.00	21.34		B	N
ANISOU	4779	N4	STU	B	1	2808	2603	2696	-37	-128	-1	B	N
ATOM	4781	C28	STU	B	1	-3.490	5.392	12.292	1.00	28.00		B	C
ANISOU	4781	C28	STU	B	1	3560	3500	3577	92	72	35	B	C
ATOM	4785	N	VAL	C	1	-4.768	14.053	8.328	0.80	35.17		C	N
ANISOU	4785	N	VAL	C	1	4423	4451	4489	7	-2	-30	C	N
ATOM	4787	CA	VAL	C	1	-5.289	15.425	8.019	0.80	34.57		C	C
ANISOU	4787	CA	VAL	C	1	4345	4381	4407	-2	-16	-7	C	C
ATOM	4789	CB	VAL	C	1	-5.982	16.066	9.179	0.00	20.00		C	C
ANISOU	4789	CB	VAL	C	1	2533	2533	2533	0	0	0	C	C
ATOM	4791	CG1	VAL	C	1	-6.577	17.405	8.749	0.00	20.00		C	C
ANISOU	4791	CG1	VAL	C	1	2533	2533	2533	0	0	0	C	C
ATOM	4795	CG2	VAL	C	1	-7.087	15.177	9.715	0.00	20.00		C	C
ANISOU	4795	CG2	VAL	C	1	2533	2533	2533	0	0	0	C	C
ATOM	4799	C	VAL	C	1	-4.186	16.328	7.466	0.80	34.42		C	C
ANISOU	4799	C	VAL	C	1	4317	4368	4390	9	-2	-21	C	C
ATOM	4800	O	VAL	C	1	-3.947	17.425	7.974	0.80	34.34		C	O
ANISOU	4800	O	VAL	C	1	4252	4402	4391	-4	-19	-35	C	O
ATOM	4803	N	TYR	C	2	-3.487	15.846	6.447	0.80	34.29		C	N
ANISOU	4803	N	TYR	C	2	4337	4360	4330	-8	-30	-11	C	N
ATOM	4805	CA	TYR	C	2	-2.410	16.610	5.828	0.80	34.20		C	C
ANISOU	4805	CA	TYR	C	2	4336	4340	4316	-10	-21	-16	C	C
ATOM	4807	CB	TYR	C	2	-1.366	15.633	5.325	0.80	34.15		C	C
ANISOU	4807	CB	TYR	C	2	4342	4337	4293	-16	-28	4	C	C
ATOM	4810	CG	TYR	C	2	-0.891	14.703	6.415	0.80	33.45		C	C
ANISOU	4810	CG	TYR	C	2	4257	4221	4228	4	-47	10	C	C
ATOM	4811	CD1	TYR	C	2	0.169	15.053	7.241	0.80	32.49		C	C
ANISOU	4811	CD1	TYR	C	2	4146	4119	4079	-3	19	27	C	C

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ATOM	4813	CE1	TYR	C	2	0.610	14.187	8.260	0.80	31.45		C	C
ANISOU	4813	CE1	TYR	C	2	4052	3967	3929	67	11	-31	C	C
ATOM	4815	CZ	TYR	C	2	-0.037	12.978	8.449	0.80	33.11		C	C
ANISOU	4815	CZ	TYR	C	2	4217	4208	4154	-28	16	23	C	C
ATOM	4816	OH	TYR	C	2	0.375	12.095	9.436	0.80	34.20		C	O
ANISOU	4816	OH	TYR	C	2	4337	4403	4253	0	-43	30	C	O
ATOM	4818	CE2	TYR	C	2	-1.095	12.621	7.643	0.80	33.83		C	C
ANISOU	4818	CE2	TYR	C	2	4288	4268	4297	-48	-64	36	C	C
ATOM	4820	CD2	TYR	C	2	-1.523	13.485	6.639	0.80	33.95		C	C
ANISOU	4820	CD2	TYR	C	2	4297	4316	4284	-51	-63	39	C	C
ATOM	4822	C	TYR	C	2	-2.864	17.544	4.698	0.80	34.84		C	C
ANISOU	4822	C	TYR	C	2	4424	4410	4400	-3	-48	-10	C	C
ATOM	4823	O	TYR	C	2	-3.461	17.096	3.709	0.80	35.34		C	O
ANISOU	4823	O	TYR	C	2	4494	4498	4434	-13	-109	-17	C	O
ATOM	4824	N	GLU	C	3	-2.557	18.836	4.825	0.80	35.12		C	N
ANISOU	4824	N	GLU	C	3	4454	4453	4434	-10	-36	-4	C	N
ATOM	4826	CA	GLU	C	3	-2.971	19.819	3.818	0.80	35.75		C	C
ANISOU	4826	CA	GLU	C	3	4540	4511	4533	2	-16	14	C	C
ATOM	4828	CB	GLU	C	3	-4.282	20.485	4.244	0.80	36.25		C	C
ANISOU	4828	CB	GLU	C	3	4584	4579	4611	18	-3	19	C	C
ATOM	4831	CG	GLU	C	3	-4.126	21.585	5.291	0.80	36.63		C	C
ANISOU	4831	CG	GLU	C	3	4608	4672	4638	-9	-31	-26	C	C
ATOM	4834	CD	GLU	C	3	-5.437	22.302	5.611	0.80	38.16		C	C
ANISOU	4834	CD	GLU	C	3	4747	4911	4840	48	4	-21	C	C
ATOM	4835	OE1	GLU	C	3	-6.454	21.612	5.865	0.80	38.38		C	O
ANISOU	4835	OE1	GLU	C	3	4820	5002	4760	30	-14	64	C	O
ATOM	4836	OE2	GLU	C	3	-5.444	23.556	5.612	0.80	39.38		C	O
ANISOU	4836	OE2	GLU	C	3	4936	5071	4955	90	-20	2	C	O
ATOM	4837	C	GLU	C	3	-1.909	20.887	3.537	0.80	36.16		C	C
ANISOU	4837	C	GLU	C	3	4574	4567	4598	-2	-24	18	C	C
ATOM	4838	O	GLU	C	3	-0.970	21.057	4.313	0.80	35.14		C	O
ANISOU	4838	O	GLU	C	3	4499	4387	4465	22	-44	6	C	O
ATOM	4839	N	SER	C	4	-2.118	21.656	2.462	1.00	37.08		C	N
ANISOU	4839	N	SER	C	4	4707	4701	4681	-6	-21	31	C	N
ATOM	4841	CA	SER	C	4	-1.132	22.639	1.993	1.00	37.93		C	C
ANISOU	4841	CA	SER	C	4	4806	4801	4804	-15	-22	27	C	C
ATOM	4843	CB	SER	C	4	0.081	21.978	1.315	1.00	38.32		C	C
ANISOU	4843	CB	SER	C	4	4835	4878	4846	-2	-14	-6	C	C
ATOM	4846	OG	SER	C	4	-0.217	21.470	0.020	1.00	40.27		C	O
ANISOU	4846	OG	SER	C	4	5186	5147	4965	4	-57	-28	C	O
ATOM	4848	C	SER	C	4	-1.767	23.634	1.026	1.00	38.18		C	C
ANISOU	4848	C	SER	C	4	4810	4850	4846	1	-41	39	C	C
ATOM	4849	O	SER	C	4	-2.974	23.601	0.795	1.00	38.78		C	O
ANISOU	4849	O	SER	C	4	4845	4934	4954	-32	-55	28	C	O
ATOM	4850	O	HOH	W	1	10.491	17.690	20.594	1.00	14.93		W	O
ANISOU	4850	O	HOH	W	1	1497	2130	2042	144	-42	200	W	O
ATOM	4853	O	HOH	W	2	-5.104	18.880	9.847	1.00	19.28		W	O
ANISOU	4853	O	HOH	W	2	2233	2984	2105	-182	117	-132	W	O
ATOM	4856	O	HOH	W	3	-4.305	23.207	16.827	1.00	15.20		W	O
ANISOU	4856	O	HOH	W	3	1584	2182	2008	170	-92	-65	W	O
ATOM	4859	O	HOH	W	4	-7.759	24.238	20.709	1.00	14.64		W	O
ANISOU	4859	O	HOH	W	4	1885	1943	1734	141	69	-2	W	O
ATOM	4862	O	HOH	W	5	-4.764	11.647	15.394	1.00	16.80		W	O
ANISOU	4862	O	HOH	W	5	1876	2046	2458	51	-57	33	W	O
ATOM	4865	O	HOH	W	6	13.202	23.121	20.612	1.00	17.14		W	O
ANISOU	4865	O	HOH	W	6	1699	2531	2282	-25	-227	22	W	O
ATOM	4868	O	HOH	W	7	4.065	17.758	16.308	1.00	15.54		W	O
ANISOU	4868	O	HOH	W	7	1738	2183	1980	34	89	-92	W	O
ATOM	4871	O	HOH	W	8	7.187	12.676	12.184	1.00	18.66		W	O
ANISOU	4871	O	HOH	W	8	2616	2352	2122	119	158	-89	W	O
ATOM	4874	O	HOH	W	9	8.255	-5.714	18.697	1.00	19.47		W	O
ANISOU	4874	O	HOH	W	9	2964	2153	2278	110	-114	-129	W	O

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ATOM	4877	O	HOH	W	10	20.540	19.977	18.271	1.00	20.05		W	O
ANISOU	4877	O	HOH	W	10	2090	2696	2830	-105	-153	-32	W	O
ATOM	4880	O	HOH	W	11	2.996	-5.718	19.792	1.00	21.07		W	O
ANISOU	4880	O	HOH	W	11	2699	2355	2949	152	-116	-32	W	O
ATOM	4883	O	HOH	W	12	17.319	23.179	13.145	1.00	19.75		W	O
ANISOU	4883	O	HOH	W	12	1838	3033	2633	301	-19	179	W	O
ATOM	4886	O	HOH	W	13	-4.391	32.837	21.222	1.00	16.89		W	O
ANISOU	4886	O	HOH	W	13	2046	1772	2598	105	2	-81	W	O
ATOM	4889	O	HOH	W	14	11.564	10.957	29.744	1.00	19.45		W	O
ANISOU	4889	O	HOH	W	14	2425	2721	2242	231	-267	2	W	O
ATOM	4892	O	HOH	W	15	2.256	-9.964	17.889	1.00	18.04		W	O
ANISOU	4892	O	HOH	W	15	2061	2495	2296	-380	17	62	W	O
ATOM	4895	O	HOH	W	16	-3.551	24.441	14.505	1.00	18.08		W	O
ANISOU	4895	O	HOH	W	16	1715	2575	2577	211	164	-90	W	O
ATOM	4898	O	HOH	W	17	-14.724	16.365	22.863	1.00	23.83		W	O
ANISOU	4898	O	HOH	W	17	2800	3293	2959	60	139	143	W	O
ATOM	4901	O	HOH	W	18	9.801	16.513	34.031	1.00	20.33		W	O
ANISOU	4901	O	HOH	W	18	2517	2784	2422	12	-219	222	W	O
ATOM	4904	O	HOH	W	19	2.978	22.134	16.268	1.00	18.41		W	O
ANISOU	4904	O	HOH	W	19	2243	2349	2401	14	-416	171	W	O
ATOM	4907	O	HOH	W	20	24.427	23.002	20.875	1.00	23.43		W	O
ANISOU	4907	O	HOH	W	20	2713	3054	3132	-37	4	233	W	O
ATOM	4910	O	HOH	W	21	-2.043	33.503	14.347	1.00	23.44		W	O
ANISOU	4910	O	HOH	W	21	2780	3331	2792	-76	-19	178	W	O
ATOM	4913	O	HOH	W	22	3.470	4.519	33.412	1.00	23.34		W	O
ANISOU	4913	O	HOH	W	22	3198	2744	2925	125	-272	376	W	O
ATOM	4916	O	HOH	W	23	11.671	21.553	28.849	1.00	25.28		W	O
ANISOU	4916	O	HOH	W	23	2929	3633	3042	210	-73	-175	W	O
ATOM	4919	O	HOH	W	24	-4.761	35.267	19.955	1.00	19.59		W	O
ANISOU	4919	O	HOH	W	24	2859	1952	2632	149	-143	70	W	O
ATOM	4922	O	HOH	W	25	11.481	24.404	22.321	1.00	21.15		W	O
ANISOU	4922	O	HOH	W	25	2221	2694	3121	249	-77	-47	W	O
ATOM	4925	O	HOH	W	26	17.232	29.203	18.157	1.00	23.19		W	O
ANISOU	4925	O	HOH	W	26	2701	2679	3428	14	-199	-34	W	O
ATOM	4928	O	HOH	W	27	-13.747	18.215	17.130	0.50	17.29		W	O
ANISOU	4928	O	HOH	W	27	1736	2851	1979	9	51	512	W	O
ATOM	4931	O	HOH	W	28	8.831	25.050	30.493	1.00	24.43		W	O
ANISOU	4931	O	HOH	W	28	3240	2988	3054	-111	-370	-169	W	O
ATOM	4934	O	HOH	W	29	-4.593	28.342	25.573	1.00	21.83		W	O
ANISOU	4934	O	HOH	W	29	3095	2620	2578	385	39	-72	W	O
ATOM	4937	O	HOH	W	30	16.273	24.864	10.099	1.00	25.38		W	O
ANISOU	4937	O	HOH	W	30	2773	3646	3223	-156	263	-11	W	O
ATOM	4940	O	HOH	W	31	1.984	2.562	34.561	1.00	28.52		W	O
ANISOU	4940	O	HOH	W	31	3736	3267	3833	-2	-63	273	W	O
ATOM	4943	O	HOH	W	32	18.556	-12.417	20.505	1.00	22.88		W	O
ANISOU	4943	O	HOH	W	32	2490	3165	3036	-290	-80	320	W	O
ATOM	4946	O	HOH	W	33	9.931	22.519	30.749	1.00	21.34		W	O
ANISOU	4946	O	HOH	W	33	2847	2756	2505	-73	-174	-42	W	O
ATOM	4949	O	HOH	W	34	15.785	7.070	27.244	1.00	27.87		W	O
ANISOU	4949	O	HOH	W	34	3171	3743	3674	199	-375	65	W	O
ATOM	4952	O	HOH	W	35	21.606	29.472	12.497	1.00	29.75		W	O
ANISOU	4952	O	HOH	W	35	3842	3462	3998	211	-20	257	W	O
ATOM	4955	O	HOH	W	36	4.084	-8.154	18.892	1.00	19.86		W	O
ANISOU	4955	O	HOH	W	36	2517	2169	2860	-138	-96	-54	W	O
ATOM	4958	O	HOH	W	37	14.363	20.892	21.951	1.00	21.92		W	O
ANISOU	4958	O	HOH	W	37	2439	3125	2763	-172	-187	258	W	O
ATOM	4961	O	HOH	W	38	-5.998	0.628	18.068	1.00	22.30		W	O
ANISOU	4961	O	HOH	W	38	2469	2647	3355	-178	-148	-152	W	O
ATOM	4964	O	HOH	W	39	13.128	17.718	28.124	1.00	21.94		W	O
ANISOU	4964	O	HOH	W	39	2898	3039	2397	72	-141	-103	W	O
ATOM	4967	O	HOH	W	40	2.120	-6.182	22.234	1.00	21.09		W	O
ANISOU	4967	O	HOH	W	40	2839	2292	2880	-208	14	-302	W	O

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ATOM	4970	O	HOH	W	41	3.175	31.298	18.185	1.00	21.87		W	O
ANISOU	4970	O	HOH	W	41	3223	2075	3011	72	348	101	W	O
ATOM	4973	O	HOH	W	42	9.059	-12.510	3.659	1.00	29.08		W	O
ANISOU	4973	O	HOH	W	42	3962	4082	3005	-44	-112	-29	W	O
ATOM	4976	O	HOH	W	43	2.374	6.789	33.008	1.00	21.44		W	O
ANISOU	4976	O	HOH	W	43	3021	2541	2583	-79	20	73	W	O
ATOM	4979	O	HOH	W	44	7.833	20.558	16.285	1.00	21.57		W	O
ANISOU	4979	O	HOH	W	44	2899	2489	2807	-146	120	-25	W	O
ATOM	4982	O	HOH	W	45	-12.896	20.048	18.738	0.50	16.48		W	O
ANISOU	4982	O	HOH	W	45	1820	2219	2223	-14	23	221	W	O
ATOM	4985	O	HOH	W	46	17.031	15.752	10.447	1.00	23.31		W	O
ANISOU	4985	O	HOH	W	46	2439	3607	2809	-72	177	-458	W	O
ATOM	4988	O	HOH	W	47	-8.368	11.387	16.200	1.00	24.44		W	O
ANISOU	4988	O	HOH	W	47	2415	2877	3993	-102	-213	86	W	O
ATOM	4991	O	HOH	W	48	5.138	11.786	9.605	1.00	25.08		W	O
ANISOU	4991	O	HOH	W	48	3011	3040	3477	54	58	86	W	O
ATOM	4994	O	HOH	W	49	-15.174	33.676	22.184	1.00	27.77		W	O
ANISOU	4994	O	HOH	W	49	3565	3430	3554	165	-120	-37	W	O
ATOM	4997	O	HOH	W	50	4.604	-16.008	10.133	1.00	23.91		W	O
ANISOU	4997	O	HOH	W	50	2904	2790	3389	-94	-39	157	W	O
ATOM	5000	O	HOH	W	51	1.096	7.858	10.304	1.00	25.08		W	O
ANISOU	5000	O	HOH	W	51	3261	3331	2936	-10	-144	207	W	O
ATOM	5003	O	HOH	W	52	-8.720	35.457	13.283	1.00	28.20		W	O
ANISOU	5003	O	HOH	W	52	3996	3408	3308	40	14	223	W	O
ATOM	5006	O	HOH	W	53	5.253	20.571	15.450	1.00	25.25		W	O
ANISOU	5006	O	HOH	W	53	3875	2619	3096	97	605	160	W	O
ATOM	5009	O	HOH	W	54	4.312	37.543	29.036	1.00	27.93		W	O
ANISOU	5009	O	HOH	W	54	3736	3092	3781	-146	-125	9	W	O
ATOM	5012	O	HOH	W	55	5.633	6.850	35.699	1.00	32.55		W	O
ANISOU	5012	O	HOH	W	55	4354	4415	3597	233	-166	536	W	O
ATOM	5015	O	HOH	W	56	10.874	28.796	23.910	1.00	32.52		W	O
ANISOU	5015	O	HOH	W	56	3855	4126	4375	-98	-34	70	W	O
ATOM	5018	O	HOH	W	57	0.042	15.580	13.754	1.00	26.03		W	O
ANISOU	5018	O	HOH	W	57	3263	3344	3283	113	113	-10	W	O
ATOM	5021	O	HOH	W	58	8.278	4.631	14.529	1.00	26.70		W	O
ANISOU	5021	O	HOH	W	58	3430	2917	3795	125	279	111	W	O
ATOM	5024	O	HOH	W	59	20.943	14.373	20.314	1.00	35.15		W	O
ANISOU	5024	O	HOH	W	59	4282	4375	4696	186	163	116	W	O
ATOM	5027	O	HOH	W	60	-13.285	13.032	28.869	1.00	31.05		W	O
ANISOU	5027	O	HOH	W	60	3874	4215	3707	106	318	10	W	O
ATOM	5030	O	HOH	W	61	-4.305	-2.442	11.520	1.00	26.11		W	O
ANISOU	5030	O	HOH	W	61	3409	3257	3251	-69	-123	-122	W	O
ATOM	5033	O	HOH	W	62	-3.391	31.203	14.593	1.00	24.23		W	O
ANISOU	5033	O	HOH	W	62	2778	3373	3052	-107	-75	21	W	O
ATOM	5036	O	HOH	W	63	22.700	30.635	17.586	1.00	27.92		W	O
ANISOU	5036	O	HOH	W	63	3393	3520	3692	22	123	-12	W	O
ATOM	5039	O	HOH	W	64	-12.479	30.568	12.259	1.00	24.77		W	O
ANISOU	5039	O	HOH	W	64	2877	3065	3468	197	-235	225	W	O
ATOM	5042	O	HOH	W	65	-7.643	25.210	4.958	1.00	30.89		W	O
ANISOU	5042	O	HOH	W	65	3950	4330	3457	-25	159	-25	W	O
ATOM	5045	O	HOH	W	66	11.206	23.203	24.871	1.00	26.27		W	O
ANISOU	5045	O	HOH	W	66	3632	3186	3160	-26	249	83	W	O
ATOM	5048	O	HOH	W	67	17.820	-9.732	20.513	1.00	26.98		W	O
ANISOU	5048	O	HOH	W	67	3532	3320	3400	6	54	46	W	O
ATOM	5051	O	HOH	W	68	4.970	-15.097	5.301	1.00	32.16		W	O
ANISOU	5051	O	HOH	W	68	4424	3872	3923	-107	-55	-49	W	O
ATOM	5054	O	HOH	W	69	17.186	22.896	20.871	1.00	25.84		W	O
ANISOU	5054	O	HOH	W	69	3156	3258	3402	108	91	82	W	O
ATOM	5057	O	HOH	W	70	-16.758	18.893	19.258	1.00	32.66		W	O
ANISOU	5057	O	HOH	W	70	3910	4415	4082	-56	-447	-10	W	O
ATOM	5060	O	HOH	W	71	2.285	-3.148	29.871	1.00	27.26		W	O
ANISOU	5060	O	HOH	W	71	3834	3259	3262	38	-261	-36	W	O



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ATOM	5063	O	HOH	W	72	-4.633	-3.618	16.105	1.00	27.03		W	O
ANISOU	5063	O	HOH	W	72	3489	3304	3477	97	10	-169	W	O
ATOM	5066	O	HOH	W	73	-14.703	19.351	22.869	1.00	27.02		W	O
ANISOU	5066	O	HOH	W	73	3480	3645	3139	302	-136	-80	W	O
ATOM	5069	O	HOH	W	74	-12.527	17.594	37.264	1.00	33.24		W	O
ANISOU	5069	O	HOH	W	74	4123	4299	4207	21	338	-74	W	O
ATOM	5072	O	HOH	W	75	-6.481	-2.797	19.675	1.00	30.43		W	O
ANISOU	5072	O	HOH	W	75	3413	3939	4206	-116	16	-28	W	O
ATOM	5075	O	HOH	W	76	0.920	13.283	43.125	1.00	32.41		W	O
ANISOU	5075	O	HOH	W	76	4315	4211	3785	45	-33	69	W	O
ATOM	5078	O	HOH	W	77	-6.578	8.995	12.075	1.00	34.38		W	O
ANISOU	5078	O	HOH	W	77	4353	4121	4586	6	-87	26	W	O
ATOM	5081	O	HOH	W	78	-11.091	17.261	12.025	1.00	26.49		W	O
ANISOU	5081	O	HOH	W	78	3254	3544	3266	-89	42	-65	W	O
ATOM	5084	O	HOH	W	79	5.139	21.529	35.802	1.00	28.39		W	O
ANISOU	5084	O	HOH	W	79	4163	3593	3028	-45	0	-138	W	O
ATOM	5087	O	HOH	W	80	3.158	-11.421	15.824	1.00	23.13		W	O
ANISOU	5087	O	HOH	W	80	2884	2942	2962	-297	-53	-168	W	O
ATOM	5090	O	HOH	W	81	-5.643	-0.574	13.193	1.00	34.46		W	O
ANISOU	5090	O	HOH	W	81	4330	4504	4258	142	-28	0	W	O
ATOM	5093	O	HOH	W	82	4.672	-11.004	13.596	1.00	26.34		W	O
ANISOU	5093	O	HOH	W	82	3196	3310	3500	-114	48	-146	W	O
ATOM	5096	O	HOH	W	83	20.450	19.142	11.867	1.00	25.02		W	O
ANISOU	5096	O	HOH	W	83	2710	3776	3018	-393	201	-88	W	O
ATOM	5099	O	HOH	W	84	-8.067	37.642	14.370	1.00	37.15		W	O
ANISOU	5099	O	HOH	W	84	4860	4319	4933	-78	7	10	W	O
ATOM	5102	O	HOH	W	85	2.015	34.822	15.146	1.00	34.41		W	O
ANISOU	5102	O	HOH	W	85	4082	4578	4412	-12	-20	10	W	O
ATOM	5105	O	HOH	W	86	6.473	-5.495	20.732	1.00	29.56		W	O
ANISOU	5105	O	HOH	W	86	3873	3579	3779	319	215	65	W	O
ATOM	5108	O	HOH	W	87	-0.706	0.130	34.968	1.00	30.70		W	O
ANISOU	5108	O	HOH	W	87	4218	3877	3568	-110	-19	124	W	O
ATOM	5111	O	HOH	W	88	7.087	38.936	10.894	1.00	58.35		W	O
ANISOU	5111	O	HOH	W	88	7426	7292	7450	29	-35	-9	W	O
ATOM	5114	O	HOH	W	89	7.751	19.798	6.032	0.50	22.53		W	O
ANISOU	5114	O	HOH	W	89	2713	3093	2755	-24	-10	83	W	O
ATOM	5117	O	HOH	W	90	12.779	-14.495	4.340	1.00	30.23		W	O
ANISOU	5117	O	HOH	W	90	4182	3723	3579	-57	65	-93	W	O
ATOM	5120	O	HOH	W	91	-11.783	9.115	25.711	1.00	27.11		W	O
ANISOU	5120	O	HOH	W	91	3223	3442	3632	-131	-128	248	W	O
ATOM	5123	O	HOH	W	92	10.090	8.776	5.976	1.00	32.59		W	O
ANISOU	5123	O	HOH	W	92	3943	4166	4273	-18	-16	-6	W	O
ATOM	5126	O	HOH	W	93	-12.950	35.978	20.532	1.00	30.92		W	O
ANISOU	5126	O	HOH	W	93	3726	3945	4076	214	75	2	W	O
ATOM	5129	O	HOH	W	94	17.340	18.377	9.174	1.00	36.48		W	O
ANISOU	5129	O	HOH	W	94	4507	4709	4645	-91	-4	141	W	O
ATOM	5132	O	HOH	W	95	-14.945	20.445	20.269	1.00	28.28		W	O
ANISOU	5132	O	HOH	W	95	3628	3426	3689	90	-230	79	W	O
ATOM	5135	O	HOH	W	96	17.781	-19.001	17.680	1.00	28.18		W	O
ANISOU	5135	O	HOH	W	96	3147	3909	3648	149	-88	-76	W	O
ATOM	5138	O	HOH	W	97	-5.958	-1.212	15.774	1.00	27.45		W	O
ANISOU	5138	O	HOH	W	97	3552	3451	3425	61	-93	76	W	O
ATOM	5141	O	HOH	W	98	22.128	-17.988	19.179	1.00	35.73		W	O
ANISOU	5141	O	HOH	W	98	4460	4594	4520	-32	111	-44	W	O
ATOM	5144	O	HOH	W	99	19.900	-6.433	0.856	0.50	34.08		W	O
ANISOU	5144	O	HOH	W	99	4376	4265	4305	102	32	-71	W	O
ATOM	5147	O	HOH	W	100	20.051	-11.519	2.320	1.00	40.99		W	O
ANISOU	5147	O	HOH	W	100	5329	5241	5004	-62	-7	-46	W	O
ATOM	5150	O	HOH	W	101	15.347	14.169	9.110	1.00	34.53		W	O
ANISOU	5150	O	HOH	W	101	4693	4209	4217	49	-112	-36	W	O
ATOM	5153	O	HOH	W	102	-9.117	0.988	31.718	1.00	29.24		W	O
ANISOU	5153	O	HOH	W	102	3331	3471	4307	-178	71	282	W	O

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ATOM	5156	O	HOH	W	103	3.763	32.808	15.980	1.00	31.99		W	O
ANISOU	5156	O	HOH	W	103	4476	3441	4235	204	349	140	W	O
ATOM	5159	O	HOH	W	104	-4.229	2.698	34.476	0.50	23.98		W	O
ANISOU	5159	O	HOH	W	104	2978	3078	3053	173	166	236	W	O
ATOM	5162	O	HOH	W	105	16.896	26.612	12.018	1.00	29.54		W	O
ANISOU	5162	O	HOH	W	105	3594	3819	3808	-13	-9	112	W	O
ATOM	5165	O	HOH	W	106	-4.393	1.123	9.723	1.00	33.40		W	O
ANISOU	5165	O	HOH	W	106	4329	4093	4267	11	-119	-11	W	O
ATOM	5168	O	HOH	W	107	-16.650	15.340	24.236	1.00	33.63		W	O
ANISOU	5168	O	HOH	W	107	4088	4317	4372	-379	111	72	W	O
ATOM	5171	O	HOH	W	108	15.267	3.599	17.100	1.00	32.05		W	O
ANISOU	5171	O	HOH	W	108	4257	4153	3766	-198	131	-70	W	O
ATOM	5174	O	HOH	W	109	5.696	3.258	32.505	1.00	35.80		W	O
ANISOU	5174	O	HOH	W	109	4834	4289	4479	16	77	171	W	O
ATOM	5177	O	HOH	W	110	-3.077	20.310	35.507	1.00	37.71		W	O
ANISOU	5177	O	HOH	W	110	4780	4734	4813	-89	18	65	W	O
ATOM	5180	O	HOH	W	111	1.016	-14.485	7.227	1.00	29.60		W	O
ANISOU	5180	O	HOH	W	111	3913	3847	3485	-186	-82	-26	W	O
ATOM	5183	O	HOH	W	112	11.673	-5.640	-7.085	1.00	48.30		W	O
ANISOU	5183	O	HOH	W	112	6224	6092	6033	27	3	33	W	O
ATOM	5186	O	HOH	W	113	11.646	8.183	29.553	1.00	27.43		W	O
ANISOU	5186	O	HOH	W	113	3724	3215	3482	47	71	-183	W	O
ATOM	5189	O	HOH	W	114	-3.801	26.629	12.705	1.00	30.98		W	O
ANISOU	5189	O	HOH	W	114	3894	3909	3965	80	23	223	W	O
ATOM	5192	O	HOH	W	115	-10.050	6.411	36.534	1.00	31.82		W	O
ANISOU	5192	O	HOH	W	115	3961	3911	4218	-116	271	186	W	O
ATOM	5195	O	HOH	W	116	25.347	30.027	14.572	1.00	28.52		W	O
ANISOU	5195	O	HOH	W	116	3384	3578	3874	-144	155	70	W	O
ATOM	5198	O	HOH	W	117	-7.180	25.097	37.761	1.00	32.15		W	O
ANISOU	5198	O	HOH	W	117	4497	3766	3951	185	9	114	W	O
ATOM	5201	O	HOH	W	118	2.937	-0.779	31.540	1.00	45.58		W	O
ANISOU	5201	O	HOH	W	118	5863	5704	5749	87	-32	-32	W	O
ATOM	5204	O	HOH	W	119	20.162	-11.330	13.435	1.00	36.48		W	O
ANISOU	5204	O	HOH	W	119	4478	4923	4460	-90	146	-41	W	O
ATOM	5207	O	HOH	W	120	19.211	-16.114	0.911	1.00	40.04		W	O
ANISOU	5207	O	HOH	W	120	5282	5136	4794	1	-49	-23	W	O
ATOM	5210	O	HOH	W	121	-12.796	7.141	34.613	1.00	39.05		W	O
ANISOU	5210	O	HOH	W	121	4706	5055	5076	43	122	-4	W	O
ATOM	5213	O	HOH	W	122	-13.375	16.123	11.503	1.00	39.74		W	O
ANISOU	5213	O	HOH	W	122	4770	5180	5147	-16	59	-112	W	O
ATOM	5216	O	HOH	W	123	19.394	18.745	26.283	1.00	35.53		W	O
ANISOU	5216	O	HOH	W	123	4116	4561	4822	-78	-11	-64	W	O
ATOM	5219	O	HOH	W	124	11.839	24.358	27.133	1.00	34.30		W	O
ANISOU	5219	O	HOH	W	124	4139	4375	4515	-9	-27	47	W	O
ATOM	5222	O	HOH	W	125	-8.819	15.707	11.225	1.00	33.15		W	O
ANISOU	5222	O	HOH	W	125	3997	4156	4442	-48	-15	-71	W	O
ATOM	5225	O	HOH	W	126	10.928	26.148	28.878	1.00	43.90		W	O
ANISOU	5225	O	HOH	W	126	5634	5485	5560	-133	-92	1	W	O
ATOM	5228	O	HOH	W	127	-13.468	9.136	27.694	1.00	38.10		W	O
ANISOU	5228	O	HOH	W	127	4465	5059	4949	-100	71	42	W	O
ATOM	5231	O	HOH	W	128	2.099	19.284	39.596	1.00	39.47		W	O
ANISOU	5231	O	HOH	W	128	5252	5111	4634	46	-14	-82	W	O
ATOM	5234	O	HOH	W	129	18.790	-4.143	15.068	1.00	40.27		W	O
ANISOU	5234	O	HOH	W	129	5078	5119	5102	57	49	38	W	O
ATOM	5237	O	HOH	W	130	1.236	3.179	37.148	1.00	35.26		W	O
ANISOU	5237	O	HOH	W	130	4447	4450	4498	39	-159	61	W	O
ATOM	5240	O	HOH	W	131	5.534	33.735	20.231	1.00	43.62		W	O
ANISOU	5240	O	HOH	W	131	5355	5659	5559	12	60	161	W	O
ATOM	5243	O	HOH	W	132	-12.128	6.258	25.491	0.50	23.14		W	O
ANISOU	5243	O	HOH	W	132	2757	2883	3151	130	-21	104	W	O
ATOM	5246	O	HOH	W	133	14.538	22.863	24.178	1.00	30.21		W	O
ANISOU	5246	O	HOH	W	133	3807	4048	3622	167	-38	1	W	O

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Figure 1A – 83

ATOM	5249	O	HOH	W	134	-17.960	16.544	11.307	1.00	36.63	W	O	
ANISOU	5249	O	HOH	W	134	4350	4760	4808	-221	109	-191	W	O
ATOM	5252	O	HOH	W	135	6.012	0.090	30.579	1.00	50.99	W	O	
ANISOU	5252	O	HOH	W	135	6608	6402	6364	39	1	2	W	O
ATOM	5255	O	HOH	W	136	-15.486	16.695	18.245	1.00	32.79	W	O	
ANISOU	5255	O	HOH	W	136	4062	4196	4200	-92	-71	-29	W	O
ATOM	5258	O	HOH	W	137	-0.044	18.142	38.644	1.00	30.61	W	O	
ANISOU	5258	O	HOH	W	137	4266	3768	3596	-19	227	-89	W	O
ATOM	5261	O	HOH	W	138	-13.137	5.816	27.720	0.50	24.39	W	O	
ANISOU	5261	O	HOH	W	138	3024	3061	3182	159	15	124	W	O
ATOM	5264	O	HOH	W	139	7.671	22.534	36.188	1.00	34.40	W	O	
ANISOU	5264	O	HOH	W	139	4719	4275	4074	-140	-30	-4	W	O
ATOM	5267	O	HOH	W	140	16.724	20.401	25.120	1.00	37.10	W	O	
ANISOU	5267	O	HOH	W	140	4883	4565	4648	-163	-148	-55	W	O
ATOM	5270	O	HOH	W	141	16.194	18.879	6.514	1.00	43.73	W	O	
ANISOU	5270	O	HOH	W	141	5518	5631	5464	4	107	7	W	O
ATOM	5273	O	HOH	W	142	3.353	-15.949	7.582	1.00	28.64	W	O	
ANISOU	5273	O	HOH	W	142	4064	3108	3709	-34	-136	-100	W	O
ATOM	5276	O	HOH	W	143	14.064	11.733	29.583	1.00	31.90	W	O	
ANISOU	5276	O	HOH	W	143	3667	4236	4218	-110	-161	108	W	O
ATOM	5279	O	HOH	W	144	-6.084	11.581	12.933	1.00	30.09	W	O	
ANISOU	5279	O	HOH	W	144	3996	3733	3704	139	-369	-62	W	O
ATOM	5282	O	HOH	W	145	0.825	28.598	6.438	1.00	35.34	W	O	
ANISOU	5282	O	HOH	W	145	4710	4680	4037	105	-110	-19	W	O
ATOM	5285	O	HOH	W	146	7.046	18.188	41.655	1.00	41.79	W	O	
ANISOU	5285	O	HOH	W	146	5515	5279	5085	-1	-41	-100	W	O
ATOM	5288	O	HOH	W	147	17.472	12.458	8.935	1.00	40.76	W	O	
ANISOU	5288	O	HOH	W	147	5203	5151	5133	-66	34	39	W	O
ATOM	5291	O	HOH	W	148	20.895	-8.983	11.399	1.00	36.06	W	O	
ANISOU	5291	O	HOH	W	148	4551	4761	4387	17	55	-95	W	O
ATOM	5294	O	HOH	W	149	15.356	19.502	27.737	1.00	33.95	W	O	
ANISOU	5294	O	HOH	W	149	4030	4516	4352	52	-40	-79	W	O
ATOM	5297	O	HOH	W	150	8.309	10.619	4.946	1.00	48.48	W	O	
ANISOU	5297	O	HOH	W	150	6144	6172	6102	-19	7	-46	W	O
ATOM	5300	O	HOH	W	151	11.664	14.372	7.921	1.00	36.16	W	O	
ANISOU	5300	O	HOH	W	151	4531	4775	4431	-54	33	135	W	O
ATOM	5303	O	HOH	W	152	7.729	28.493	29.591	1.00	34.41	W	O	
ANISOU	5303	O	HOH	W	152	4395	4427	4253	-10	-39	47	W	O
ATOM	5306	O	HOH	W	153	8.813	3.879	-6.241	1.00	51.38	W	O	
ANISOU	5306	O	HOH	W	153	6512	6519	6490	22	19	27	W	O
ATOM	5309	O	HOH	W	154	7.173	-2.863	20.927	1.00	32.30	W	O	
ANISOU	5309	O	HOH	W	154	3922	4269	4079	21	-30	-62	W	O
ATOM	5312	O	HOH	W	155	-3.083	3.088	36.079	0.50	33.42	W	O	
ANISOU	5312	O	HOH	W	155	4133	4186	4376	-33	45	24	W	O
ATOM	5315	O	HOH	W	156	9.209	7.337	2.559	1.00	37.49	W	O	
ANISOU	5315	O	HOH	W	156	4729	4801	4714	-107	6	88	W	O
ATOM	5318	O	HOH	W	157	20.587	-9.503	17.607	1.00	44.34	W	O	
ANISOU	5318	O	HOH	W	157	5399	5773	5676	-49	-27	49	W	O
ATOM	5321	O	HOH	W	158	9.849	21.085	35.220	1.00	34.31	W	O	
ANISOU	5321	O	HOH	W	158	4430	4316	4290	-228	-51	-153	W	O
ATOM	5324	O	HOH	W	159	-3.994	28.379	7.850	1.00	33.18	W	O	
ANISOU	5324	O	HOH	W	159	3800	4594	4211	-4	-54	-16	W	O
ATOM	5327	O	HOH	W	160	8.181	0.696	29.938	1.00	43.36	W	O	
ANISOU	5327	O	HOH	W	160	5575	5378	5521	65	-7	75	W	O
ATOM	5330	O	HOH	W	161	10.395	32.461	9.596	1.00	38.63	W	O	
ANISOU	5330	O	HOH	W	161	4903	4857	4917	-33	191	47	W	O
ATOM	5333	O	HOH	W	162	8.923	31.515	17.203	1.00	37.00	W	O	
ANISOU	5333	O	HOH	W	162	4618	4688	4752	-83	114	2	W	O
ATOM	5336	O	HOH	W	163	23.091	-12.507	8.376	1.00	38.58	W	O	
ANISOU	5336	O	HOH	W	163	4827	5114	4717	146	109	-2	W	O
ATOM	5339	O	HOH	W	164	-7.196	-5.003	23.927	1.00	45.70	W	O	
ANISOU	5339	O	HOH	W	164	5754	5684	5923	-46	66	50	W	O

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ATOM	5342	O	HOH	W	165	12.948	31.844	17.586	1.00	41.79		W	O
ANISOU	5342	O	HOH	W	165	5362	5210	5305	22	-37	-53	W	O
ATOM	5345	O	HOH	W	166	9.747	14.633	5.508	1.00	58.80		W	O
ANISOU	5345	O	HOH	W	166	7382	7509	7450	22	66	0	W	O
ATOM	5348	O	HOH	W	167	7.934	11.481	40.968	1.00	45.05		W	O
ANISOU	5348	O	HOH	W	167	5707	5890	5518	8	26	37	W	O
ATOM	5351	O	HOH	W	168	-5.302	1.864	11.880	1.00	37.65		W	O
ANISOU	5351	O	HOH	W	168	4781	4762	4762	-78	-78	-94	W	O
ATOM	5354	O	HOH	W	169	-1.994	30.048	6.669	1.00	42.66		W	O
ANISOU	5354	O	HOH	W	169	5476	5498	5235	5	-142	115	W	O
ATOM	5357	O	HOH	W	170	5.006	11.843	6.891	1.00	44.35		W	O
ANISOU	5357	O	HOH	W	170	5866	5527	5456	-57	-80	-12	W	O
ATOM	5360	O	HOH	W	171	8.797	34.488	14.676	1.00	43.13		W	O
ANISOU	5360	O	HOH	W	171	5402	5419	5566	-46	42	-6	W	O
ATOM	5363	O	HOH	W	172	3.952	20.780	38.293	1.00	39.12		W	O
ANISOU	5363	O	HOH	W	172	5141	5244	4476	-24	76	-37	W	O
ATOM	5366	O	HOH	W	173	23.129	-16.085	16.267	1.00	45.71		W	O
ANISOU	5366	O	HOH	W	173	5733	5739	5895	34	43	32	W	O
ATOM	5369	O	HOH	W	174	-2.458	19.536	37.786	1.00	44.75		W	O
ANISOU	5369	O	HOH	W	174	5686	5668	5646	9	17	-16	W	O
ATOM	5372	O	HOH	W	175	-8.750	5.588	48.411	1.00	43.07		W	O
ANISOU	5372	O	HOH	W	175	5395	5520	5448	61	66	96	W	O
ATOM	5375	O	HOH	W	176	-4.501	22.526	37.127	1.00	32.29		W	O
ANISOU	5375	O	HOH	W	176	4283	4163	3819	-68	-99	-4	W	O
ATOM	5378	O	HOH	W	177	-16.014	34.420	18.257	1.00	34.69		W	O
ANISOU	5378	O	HOH	W	177	4193	4397	4589	40	-73	156	W	O
ATOM	5381	O	HOH	W	178	11.054	18.493	35.728	1.00	39.81		W	O
ANISOU	5381	O	HOH	W	178	4964	5184	4977	82	-91	60	W	O
ATOM	5384	O	HOH	W	179	10.816	28.661	27.786	1.00	41.40		W	O
ANISOU	5384	O	HOH	W	179	5077	5346	5304	-44	-80	-63	W	O
ATOM	5387	O	HOH	W	180	10.690	10.925	32.258	1.00	39.61		W	O
ANISOU	5387	O	HOH	W	180	4991	5144	4915	-33	55	39	W	O
ATOM	5390	O	HOH	W	181	21.127	17.964	22.018	1.00	48.14		W	O
ANISOU	5390	O	HOH	W	181	6038	6065	6186	32	-54	-23	W	O
ATOM	5393	O	HOH	W	182	11.189	22.790	33.135	1.00	29.06		W	O
ANISOU	5393	O	HOH	W	182	3795	3895	3350	-219	-273	-219	W	O
ATOM	5396	O	HOH	W	183	-0.452	-12.230	12.107	0.70	31.49		W	O
ANISOU	5396	O	HOH	W	183	4055	3801	4106	-46	-226	-86	W	O
ATOM	5399	O	HOH	W	184	7.567	9.522	2.715	1.00	47.40		W	O
ANISOU	5399	O	HOH	W	184	5996	6009	6004	16	-44	-10	W	O
ATOM	5402	O	HOH	W	185	-3.763	16.389	41.536	1.00	36.79		W	O
ANISOU	5402	O	HOH	W	185	4778	4681	4518	103	65	73	W	O
ATOM	5405	O	HOH	W	186	-1.256	26.366	6.637	1.00	37.33		W	O
ANISOU	5405	O	HOH	W	186	4898	4576	4710	-54	-3	1	W	O
ATOM	5408	O	HOH	W	187	-6.618	-5.332	12.517	1.00	41.09		W	O
ANISOU	5408	O	HOH	W	187	5129	5195	5286	-2	-72	-81	W	O
ATOM	5411	O	HOH	W	188	11.688	11.560	6.432	1.00	35.83		W	O
ANISOU	5411	O	HOH	W	188	4651	4521	4441	61	14	34	W	O
ATOM	5414	O	HOH	W	189	-12.291	18.381	8.048	1.00	52.22		W	O
ANISOU	5414	O	HOH	W	189	6536	6689	6613	-63	-21	-2	W	O
ATOM	5417	O	HOH	W	190	-17.341	18.808	31.364	0.50	36.73		W	O
ANISOU	5417	O	HOH	W	190	4637	4715	4601	21	9	-18	W	O
ATOM	5420	O	HOH	W	191	11.185	27.219	21.623	1.00	39.74		W	O
ANISOU	5420	O	HOH	W	191	4986	4969	5142	39	196	-54	W	O
ATOM	5423	O	HOH	W	192	22.930	-10.153	10.084	1.00	43.32		W	O
ANISOU	5423	O	HOH	W	192	5534	5528	5395	5	29	14	W	O
ATOM	5426	O	HOH	W	193	14.195	14.900	6.664	1.00	35.68		W	O
ANISOU	5426	O	HOH	W	193	4792	4474	4288	68	-54	-58	W	O
ATOM	5429	O	HOH	W	194	-10.297	9.163	14.690	0.70	39.50		W	O
ANISOU	5429	O	HOH	W	194	4904	5097	5006	128	41	-67	W	O
ATOM	5432	O	HOH	W	195	9.966	28.770	17.324	1.00	30.88		W	O
ANISOU	5432	O	HOH	W	195	3832	4169	3730	-47	67	141	W	O

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ATOM	5435	O	HOH	W	196	14.028	21.351	30.123	1.00	37.29		W	O
ANISOU	5435	O	HOH	W	196	4577	4853	4737	-14	-219	44	W	O
ATOM	5438	O	HOH	W	197	-13.856	-0.307	26.739	1.00	44.29		W	O
ANISOU	5438	O	HOH	W	197	5591	5576	5662	-54	90	9	W	O
ATOM	5441	O	HOH	W	198	19.207	22.246	24.335	1.00	37.77		W	O
ANISOU	5441	O	HOH	W	198	4703	4825	4823	-63	28	-74	W	O
ATOM	5444	O	HOH	W	199	-3.154	2.981	7.777	1.00	38.30		W	O
ANISOU	5444	O	HOH	W	199	4888	4769	4894	158	-53	-40	W	O
ATOM	5447	O	HOH	W	200	19.505	15.218	10.199	1.00	44.69		W	O
ANISOU	5447	O	HOH	W	200	5510	5738	5729	-9	20	-75	W	O
ATOM	5450	O	HOH	W	201	-3.198	2.143	43.619	1.00	45.18		W	O
ANISOU	5450	O	HOH	W	201	5668	5746	5753	-5	-53	128	W	O
ATOM	5453	O	HOH	W	202	2.256	-13.037	13.525	1.00	44.86		W	O
ANISOU	5453	O	HOH	W	202	5745	5550	5749	-14	0	17	W	O
ATOM	5456	O	HOH	W	203	14.000	31.186	25.550	1.00	53.16		W	O
ANISOU	5456	O	HOH	W	203	6655	6757	6785	21	-23	-10	W	O
ATOM	5459	O	HOH	W	204	-3.464	25.979	7.624	1.00	37.58		W	O
ANISOU	5459	O	HOH	W	204	4666	4834	4780	7	-36	-62	W	O
ATOM	5462	O	HOH	W	205	-5.657	-3.581	33.184	1.00	42.33		W	O
ANISOU	5462	O	HOH	W	205	5369	5333	5382	-72	86	34	W	O
ATOM	5465	O	HOH	W	206	9.242	4.647	-8.769	0.50	33.08		W	O
ANISOU	5465	O	HOH	W	206	4105	4154	4310	6	-54	-134	W	O
ATOM	5468	O	HOH	W	207	-16.836	22.274	27.090	1.00	38.92		W	O
ANISOU	5468	O	HOH	W	207	5056	4992	4740	242	1	-52	W	O
ATOM	5471	O	HOH	W	208	-9.022	8.271	11.251	1.00	43.41		W	O
ANISOU	5471	O	HOH	W	208	5364	5605	5524	-42	-74	21	W	O
ATOM	5474	O	HOH	W	209	7.559	25.032	35.271	1.00	42.48		W	O
ANISOU	5474	O	HOH	W	209	5667	5308	5165	-29	21	-9	W	O
ATOM	5477	O	HOH	W	210	9.282	10.742	34.675	1.00	39.29		W	O
ANISOU	5477	O	HOH	W	210	4909	4877	5140	91	-113	15	W	O
ATOM	5480	O	HOH	W	211	-4.305	-7.372	6.171	1.00	35.47		W	O
ANISOU	5480	O	HOH	W	211	4383	4485	4609	-114	-172	1	W	O
ATOM	5483	O	HOH	W	212	15.971	-1.673	18.376	1.00	41.60		W	O
ANISOU	5483	O	HOH	W	212	5305	5296	5205	1	-54	11	W	O
ATOM	5486	O	HOH	W	213	-5.353	-3.786	9.488	1.00	46.40		W	O
ANISOU	5486	O	HOH	W	213	5904	5844	5881	-60	-59	-115	W	O
ATOM	5489	O	HOH	W	214	17.256	2.335	19.313	1.00	53.32		W	O
ANISOU	5489	O	HOH	W	214	6712	6686	6859	19	-25	-49	W	O
ATOM	5492	O	HOH	W	215	13.971	29.783	4.832	1.00	51.81		W	O
ANISOU	5492	O	HOH	W	215	6551	6677	6455	-19	38	39	W	O
ATOM	5495	O	HOH	W	216	14.759	25.692	23.886	1.00	47.89		W	O
ANISOU	5495	O	HOH	W	216	6025	6123	6046	-60	-42	-34	W	O
ATOM	5498	O	HOH	W	217	18.255	10.574	3.198	1.00	40.31		W	O
ANISOU	5498	O	HOH	W	217	5045	5038	5230	-37	55	-22	W	O
ATOM	5501	O	HOH	W	218	23.308	-13.411	10.780	1.00	49.29		W	O
ANISOU	5501	O	HOH	W	218	6195	6354	6177	95	-14	-54	W	O
ATOM	5504	O	HOH	W	219	-11.609	15.487	7.924	1.00	57.20		W	O
ANISOU	5504	O	HOH	W	219	7183	7283	7265	-3	9	-13	W	O
ATOM	5507	O	HOH	W	220	-18.114	32.474	19.132	1.00	40.07		W	O
ANISOU	5507	O	HOH	W	220	5315	4900	5010	78	-66	-81	W	O
ATOM	5510	O	HOH	W	221	-6.926	20.420	8.232	1.00	41.29		W	O
ANISOU	5510	O	HOH	W	221	5083	5484	5121	70	-19	54	W	O
ATOM	5513	O	HOH	W	222	10.459	34.247	11.417	1.00	43.37		W	O
ANISOU	5513	O	HOH	W	222	5418	5449	5611	-89	-64	-24	W	O
ATOM	5516	O	HOH	W	223	12.427	15.100	36.876	1.00	52.63		W	O
ANISOU	5516	O	HOH	W	223	6604	6723	6668	-32	-37	-14	W	O
ATOM	5519	O	HOH	W	224	-12.039	12.315	9.086	1.00	53.41		W	O
ANISOU	5519	O	HOH	W	224	6693	6843	6756	-39	0	-65	W	O
ATOM	5522	O	HOH	W	225	26.201	-13.569	10.739	1.00	49.57		W	O
ANISOU	5522	O	HOH	W	225	6260	6287	6286	0	16	-17	W	O
ATOM	5525	O	HOH	W	226	9.916	36.578	10.094	1.00	42.36		W	O
ANISOU	5525	O	HOH	W	226	5293	5484	5316	10	25	-20	W	O

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ATOM	5528	O	HOH	W	227	-11.707	35.102	9.559	0.50	33.82		W	O
ANISOU	5528	O	HOH	W	227	4314	4355	4182	4	-56	5	W	O
ATOM	5531	O	HOH	W	228	-10.846	4.148	46.718	1.00	51.62		W	O
ANISOU	5531	O	HOH	W	228	6552	6620	6441	-39	34	41	W	O
ATOM	5534	O	HOH	W	229	4.148	30.998	31.115	1.00	37.64		W	O
ANISOU	5534	O	HOH	W	229	4893	4642	4766	-6	-34	63	W	O
ATOM	5537	O	HOH	W	230	-5.675	-5.896	7.692	1.00	51.56		W	O
ANISOU	5537	O	HOH	W	230	6618	6486	6486	49	-25	9	W	O
ATOM	5540	O	HOH	W	231	18.110	2.157	-4.441	1.00	42.90		W	O
ANISOU	5540	O	HOH	W	231	5468	5422	5408	33	92	-48	W	O
ATOM	5543	O	HOH	W	232	-17.916	17.346	31.262	0.50	28.91		W	O
ANISOU	5543	O	HOH	W	232	3675	3694	3615	-11	29	-17	W	O
ATOM	5546	O	HOH	W	233	16.856	20.252	11.180	1.00	36.75		W	O
ANISOU	5546	O	HOH	W	233	4423	4674	4866	53	-23	144	W	O
ATOM	5549	O	HOH	W	234	-5.473	18.319	41.417	1.00	44.30		W	O
ANISOU	5549	O	HOH	W	234	5780	5491	5560	36	66	-18	W	O
ATOM	5552	O	HOH	W	235	3.651	13.143	43.683	1.00	61.07		W	O
ANISOU	5552	O	HOH	W	235	7678	7748	7777	-10	-7	-20	W	O
ATOM	5555	O	HOH	W	236	19.200	10.831	21.375	1.00	43.88		W	O
ANISOU	5555	O	HOH	W	236	5716	5475	5480	48	28	-89	W	O
ATOM	5558	O	HOH	W	237	3.973	-11.813	2.738	1.00	48.05		W	O
ANISOU	5558	O	HOH	W	237	6146	6162	5948	23	-29	23	W	O
ATOM	5561	O	HOH	W	238	13.480	18.233	34.212	1.00	55.66		W	O
ANISOU	5561	O	HOH	W	238	7024	7041	7083	-36	-85	-19	W	O
ATOM	5564	O	HOH	W	239	11.228	3.316	-4.438	1.00	60.99		W	O
ANISOU	5564	O	HOH	W	239	7717	7722	7734	-14	7	6	W	O
ATOM	5567	O	HOH	W	240	5.911	8.030	7.591	1.00	40.72		W	O
ANISOU	5567	O	HOH	W	240	5395	5099	4975	-76	43	-36	W	O
ATOM	5570	O	HOH	W	241	24.419	-11.136	23.841	1.00	39.03		W	O
ANISOU	5570	O	HOH	W	241	4960	4871	4999	-167	-19	179	W	O
ATOM	5573	O	HOH	W	242	1.762	36.622	12.038	1.00	45.79		W	O
ANISOU	5573	O	HOH	W	242	5929	5576	5892	23	-36	17	W	O
ATOM	5576	O	HOH	W	243	-8.843	21.406	40.514	1.00	52.42		W	O
ANISOU	5576	O	HOH	W	243	6692	6672	6552	-17	-47	-10	W	O
ATOM	5579	O	HOH	W	244	-6.187	5.878	48.734	1.00	48.82		W	O
ANISOU	5579	O	HOH	W	244	6269	6156	6122	44	26	45	W	O
ATOM	5582	O	HOH	W	245	-15.405	12.594	26.075	1.00	39.75		W	O
ANISOU	5582	O	HOH	W	245	4759	5215	5126	12	56	-12	W	O
ATOM	5585	O	HOH	W	246	-8.342	-0.414	37.925	1.00	49.09		W	O
ANISOU	5585	O	HOH	W	246	6210	6216	6225	-46	25	22	W	O
ATOM	5588	O	HOH	W	247	-11.960	32.211	8.377	1.00	58.41		W	O
ANISOU	5588	O	HOH	W	247	7360	7432	7400	37	-61	5	W	O
ATOM	5591	O	HOH	W	248	12.785	-4.236	24.290	1.00	44.31		W	O
ANISOU	5591	O	HOH	W	248	5709	5454	5671	-38	20	48	W	O
ATOM	5594	O	HOH	W	249	12.897	13.530	4.910	1.00	36.54		W	O
ANISOU	5594	O	HOH	W	249	4820	4557	4503	67	104	-14	W	O
ATOM	5597	O	HOH	W	250	17.251	-17.824	1.626	1.00	50.16		W	O
ANISOU	5597	O	HOH	W	250	6414	6327	6315	-24	-52	46	W	O
ATOM	5600	O	HOH	W	251	6.807	25.902	32.564	1.00	44.25		W	O
ANISOU	5600	O	HOH	W	251	5748	5400	5663	9	-21	-98	W	O
ATOM	5603	O	HOH	W	252	10.725	0.285	-5.182	1.00	54.75		W	O
ANISOU	5603	O	HOH	W	252	7022	6927	6852	20	-16	6	W	O
ATOM	5606	O	HOH	W	253	8.902	6.148	12.050	1.00	23.66		W	O
ANISOU	5606	O	HOH	W	253	3277	2626	3084	228	52	-90	W	O
ATOM	5609	O	HOH	W	254	-0.282	-12.589	8.792	1.00	33.32		W	O
ANISOU	5609	O	HOH	W	254	4340	4099	4219	44	11	193	W	O
ATOM	5612	O	HOH	W	255	19.786	29.508	19.352	1.00	28.60		W	O
ANISOU	5612	O	HOH	W	255	3522	3833	3508	-6	153	-91	W	O
ATOM	5615	O	HOH	W	256	-15.696	24.114	7.334	1.00	37.11		W	O
ANISOU	5615	O	HOH	W	256	4588	4965	4546	0	-46	126	W	O
ATOM	5618	O	HOH	W	257	-7.495	3.691	44.284	1.00	56.75		W	O
ANISOU	5618	O	HOH	W	257	7215	7175	7170	3	94	25	W	O

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ATOM	5621	O	HOH	W	258	14.917	-5.447	20.112	1.00	58.33		W	O
ANISOU	5621	O	HOH	W	258	7356	7395	7412	-48	-30	6	W	O
ATOM	5624	O	HOH	W	259	13.525	4.314	21.194	1.00	30.26		W	O
ANISOU	5624	O	HOH	W	259	3646	3887	3963	-117	-7	-28	W	O
ATOM	5627	O	HOH	W	260	17.434	-4.162	17.682	1.00	42.49		W	O
ANISOU	5627	O	HOH	W	260	5383	5365	5393	-4	-116	0	W	O
ATOM	5630	O	HOH	W	261	7.001	32.824	15.864	1.00	49.12		W	O
ANISOU	5630	O	HOH	W	261	6222	6187	6254	-24	4	44	W	O
ATOM	5633	O	HOH	W	262	-16.467	16.302	20.456	1.00	37.02		W	O
ANISOU	5633	O	HOH	W	262	4772	4688	4604	-197	-31	105	W	O
ATOM	5636	O	HOH	W	263	14.083	17.232	30.526	1.00	34.38		W	O
ANISOU	5636	O	HOH	W	263	4325	4566	4172	138	-238	2	W	O
ATOM	5639	O	HOH	W	264	8.095	26.552	17.112	1.00	30.60		W	O
ANISOU	5639	O	HOH	W	264	4242	3311	4072	196	-59	153	W	O
ATOM	5642	O	HOH	W	265	12.270	5.986	-3.853	1.00	46.18		W	O
ANISOU	5642	O	HOH	W	265	5934	5865	5746	5	3	55	W	O
ATOM	5645	O	HOH	W	266	17.498	22.741	10.441	1.00	31.96		W	O
ANISOU	5645	O	HOH	W	266	3684	4277	4181	-99	-35	82	W	O
ATOM	5648	O	HOH	W	267	19.695	8.758	23.825	1.00	39.57		W	O
ANISOU	5648	O	HOH	W	267	4843	5013	5179	84	-10	-150	W	O
ATOM	5651	O	HOH	W	268	-18.101	12.092	21.777	1.00	43.80		W	O
ANISOU	5651	O	HOH	W	268	5440	5560	5642	6	50	-59	W	O
ATOM	5654	O	HOH	W	269	-17.259	10.123	20.437	1.00	61.06		W	O
ANISOU	5654	O	HOH	W	269	7754	7681	7762	35	-2	13	W	O
ATOM	5657	O	HOH	W	270	-2.320	29.291	13.034	1.00	38.05		W	O
ANISOU	5657	O	HOH	W	270	4627	4849	4981	91	-53	82	W	O
ATOM	5660	O	HOH	W	271	-15.179	17.933	33.013	1.00	44.42		W	O
ANISOU	5660	O	HOH	W	271	5564	5666	5645	122	77	26	W	O
ATOM	5663	O	HOH	W	272	-11.643	-1.804	28.045	1.00	55.05		W	O
ANISOU	5663	O	HOH	W	272	6971	6883	7059	-16	-40	28	W	O
ATOM	5666	O	HOH	W	273	18.551	16.794	30.371	1.00	43.79		W	O
ANISOU	5666	O	HOH	W	273	5543	5536	5558	-100	-20	5	W	O
ATOM	5669	O	HOH	W	274	-3.550	-7.431	3.470	1.00	56.13		W	O
ANISOU	5669	O	HOH	W	274	7068	7114	7142	1	41	-3	W	O
ATOM	5672	O	HOH	W	275	20.127	-4.517	2.619	1.00	48.33		W	O
ANISOU	5672	O	HOH	W	275	5997	6121	6243	-32	-87	-37	W	O
ATOM	5675	O	HOH	W	276	-9.403	-2.535	20.630	1.00	56.04		W	O
ANISOU	5675	O	HOH	W	276	7063	7057	7171	14	-12	-31	W	O
ATOM	5678	O	HOH	W	277	-6.187	5.806	13.792	1.00	37.07		W	O
ANISOU	5678	O	HOH	W	277	4731	4679	4672	159	-57	-122	W	O
ATOM	5681	O	HOH	W	278	8.444	22.790	39.140	1.00	51.98		W	O
ANISOU	5681	O	HOH	W	278	6671	6550	6526	29	-26	-46	W	O
ATOM	5684	O	HOH	W	279	11.656	6.475	31.878	1.00	46.34		W	O
ANISOU	5684	O	HOH	W	279	5920	5854	5830	-3	-56	-7	W	O
ATOM	5687	O	HOH	W	280	9.109	20.736	6.005	0.50	29.06		W	O
ANISOU	5687	O	HOH	W	280	3908	3482	3650	61	-31	-54	W	O
ATOM	5690	O	HOH	W	281	-8.931	1.786	40.601	1.00	59.57		W	O
ANISOU	5690	O	HOH	W	281	7535	7518	7580	-21	10	7	W	O
ATOM	5693	O	HOH	W	282	-17.530	19.338	28.910	1.00	37.28		W	O
ANISOU	5693	O	HOH	W	282	4403	4849	4912	173	155	26	W	O
ATOM	5696	O	HOH	W	283	12.884	-0.207	26.348	1.00	46.78		W	O
ANISOU	5696	O	HOH	W	283	5984	5858	5930	130	-12	-51	W	O
ATOM	5699	O	HOH	W	284	17.386	15.016	4.723	1.00	48.89		W	O
ANISOU	5699	O	HOH	W	284	6078	6248	6247	-37	-11	53	W	O
ATOM	5702	O	HOH	W	285	-12.563	20.452	6.383	1.00	43.28		W	O
ANISOU	5702	O	HOH	W	285	5559	5533	5351	-7	-97	-99	W	O
ATOM	5705	O	HOH	W	286	-4.872	3.008	41.039	1.00	53.14		W	O
ANISOU	5705	O	HOH	W	286	6833	6692	6664	-36	-18	21	W	O
ATOM	5708	O	HOH	W	287	17.552	8.815	28.054	1.00	35.66		W	O
ANISOU	5708	O	HOH	W	287	4430	4551	4566	-45	-146	94	W	O
ATOM	5711	O	HOH	W	288	-7.711	21.660	37.950	1.00	47.04		W	O
ANISOU	5711	O	HOH	W	288	6048	5965	5860	24	-20	33	W	O

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Figure 1A – 88

ATOM	5714	O	HOH	W	289	-2.805	9.102	8.672	1.00	35.74	W	O	
ANISOU	5714	O	HOH	W	289	4403	4632	4543	-26	-175	-17	W	O
ATOM	5717	O	HOH	W	290	19.977	-16.266	13.219	1.00	43.81	W	O	
ANISOU	5717	O	HOH	W	290	5534	5502	5608	125	38	-85	W	O
ATOM	5720	O	HOH	W	291	-19.529	3.936	19.692	1.00	46.33	W	O	
ANISOU	5720	O	HOH	W	291	5787	5940	5874	-25	22	-52	W	O
ATOM	5723	O	HOH	W	292	-17.457	14.268	12.882	1.00	54.27	W	O	
ANISOU	5723	O	HOH	W	292	6937	6799	6881	-32	-20	-60	W	O
ATOM	5726	O	HOH	W	293	-1.096	17.224	41.033	1.00	38.51	W	O	
ANISOU	5726	O	HOH	W	293	5219	4913	4500	-35	64	-14	W	O
ATOM	5729	O	HOH	W	294	19.393	13.048	30.807	1.00	47.68	W	O	
ANISOU	5729	O	HOH	W	294	5863	6164	6089	-33	11	-25	W	O
ATOM	5732	O	HOH	W	295	15.791	4.556	28.623	1.00	45.90	W	O	
ANISOU	5732	O	HOH	W	295	5701	5874	5865	-5	-119	65	W	O
ATOM	5735	O	HOH	W	296	12.437	11.930	9.155	1.00	40.51	W	O	
ANISOU	5735	O	HOH	W	296	5221	5093	5075	-8	-47	56	W	O
ATOM	5738	O	HOH	W	297	-3.292	-12.327	9.101	1.00	40.43	W	O	
ANISOU	5738	O	HOH	W	297	5008	5114	5238	-65	15	-82	W	O
ATOM	5741	O	HOH	W	298	20.404	-8.353	15.184	1.00	53.92	W	O	
ANISOU	5741	O	HOH	W	298	6780	6886	6820	-4	72	-55	W	O
ATOM	5744	O	HOH	W	299	15.036	12.852	-4.663	1.00	58.26	W	O	
ANISOU	5744	O	HOH	W	299	7280	7378	7476	-4	-23	-17	W	O
ATOM	5747	O	HOH	W	300	-4.391	25.858	10.248	1.00	42.24	W	O	
ANISOU	5747	O	HOH	W	300	5197	5584	5266	-3	-60	-10	W	O
ATOM	5750	O	HOH	W	301	10.256	4.216	32.314	1.00	44.79	W	O	
ANISOU	5750	O	HOH	W	301	5723	5742	5553	-16	1	75	W	O
ATOM	5753	O	HOH	W	302	11.078	1.268	22.859	1.00	25.93	W	O	
ANISOU	5753	O	HOH	W	302	3273	3346	3233	127	-23	198	W	O
ATOM	5756	O	HOH	W	303	1.104	-11.811	10.856	0.30	19.91	W	O	
ANISOU	5756	O	HOH	W	303	2860	2194	2510	-44	-11	-64	W	O
ATOM	5759	O	HOH	W	304	-7.435	35.305	10.939	1.00	47.81	W	O	
ANISOU	5759	O	HOH	W	304	5993	6185	5985	-84	-25	80	W	O
ATOM	5762	O	HOH	W	305	9.426	-16.998	6.199	1.00	50.78	W	O	
ANISOU	5762	O	HOH	W	305	6526	6356	6410	-51	91	-80	W	O
ATOM	5765	O	HOH	W	306	-16.253	-1.728	20.207	1.00	47.54	W	O	
ANISOU	5765	O	HOH	W	306	6072	5936	6056	-69	-14	-20	W	O
ATOM	5768	O	HOH	W	307	20.013	-17.547	7.289	1.00	68.65	W	O	
ANISOU	5768	O	HOH	W	307	8705	8724	8655	25	11	-7	W	O
ATOM	5771	O	HOH	W	308	14.469	-1.221	-4.717	1.00	51.82	W	O	
ANISOU	5771	O	HOH	W	308	6560	6555	6573	11	0	-44	W	O
ATOM	5774	O	HOH	W	309	-17.202	19.931	24.211	1.00	51.30	W	O	
ANISOU	5774	O	HOH	W	309	6455	6545	6488	19	-10	-85	W	O
END													



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Figure 2A - 1

	<u>Atom Type</u>	<u>Resid</u>	<u>#</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>Occ</u>	<u>B</u>	<u>Mol</u>	
ATOM	1	N	TYR A 364	23.735	-2.166	9.218	1.00	43.88	A	N
ATOM	2	CA	TYR A 364	22.526	-2.798	8.527	1.00	43.16	A	C
ATOM	3	CB	TYR A 364	22.787	-2.947	7.038	1.00	42.60	A	C
ATOM	4	CG	TYR A 364	22.391	-1.560	6.425	0.00	20.00	A	C
ATOM	5	CD1	TYR A 364	21.246	-1.335	5.667	0.00	20.00	A	C
ATOM	6	CE1	TYR A 364	21.091	-0.119	5.018	0.00	20.00	A	C
ATOM	7	CZ	TYR A 364	22.090	0.849	5.123	0.00	20.00	A	C
ATOM	8	OH	TYR A 364	21.968	2.029	4.426	0.00	20.00	A	O
ATOM	9	CE2	TYR A 364	23.201	0.633	5.913	0.00	20.00	A	C
ATOM	10	CD2	TYR A 364	23.345	-0.567	6.570	0.00	20.00	A	C
ATOM	11	C	TYR A 364	22.052	-4.162	9.033	1.00	42.40	A	C
ATOM	12	O	TYR A 364	22.840	-4.963	9.496	1.00	43.44	A	O
ATOM	13	N	LEU A 365	20.768	-4.464	8.922	1.00	39.91	A	N
ATOM	14	CA	LEU A 365	20.338	-5.777	9.293	1.00	39.75	A	C
ATOM	15	CB	LEU A 365	18.857	-5.810	9.783	1.00	39.56	A	C
ATOM	16	CG	LEU A 365	18.706	-5.437	11.273	1.00	36.18	A	C
ATOM	17	CD1	LEU A 365	19.831	-4.479	11.871	1.00	36.01	A	C
ATOM	18	CD2	LEU A 365	17.453	-4.844	11.475	1.00	30.99	A	C
ATOM	19	C	LEU A 365	20.469	-6.740	8.158	1.00	39.48	A	C
ATOM	20	O	LEU A 365	20.256	-6.399	6.999	1.00	38.82	A	O
ATOM	21	N	ASP A 366	20.707	-7.973	8.568	1.00	39.10	A	N
ATOM	22	CA	ASP A 366	20.791	-9.148	7.715	1.00	39.57	A	C
ATOM	23	CB	ASP A 366	21.674	-10.189	8.422	1.00	39.50	A	C
ATOM	24	CG	ASP A 366	21.757	-11.502	7.708	1.00	41.05	A	C
ATOM	25	OD1	ASP A 366	22.512	-12.329	8.262	1.00	40.48	A	O
ATOM	26	OD2	ASP A 366	21.101	-11.827	6.643	1.00	44.00	A	O
ATOM	27	C	ASP A 366	19.441	-9.688	7.352	1.00	39.13	A	C
ATOM	28	O	ASP A 366	18.780	-10.300	8.160	1.00	41.44	A	O
ATOM	29	N	ARG A 367	19.004	-9.478	6.136	1.00	38.85	A	N
ATOM	30	CA	ARG A 367	17.678	-9.942	5.677	1.00	37.77	A	C
ATOM	31	CB	ARG A 367	17.531	-9.813	4.107	1.00	36.81	A	C
ATOM	32	CG	ARG A 367	16.160	-10.315	3.539	1.00	32.15	A	C
ATOM	33	CD	ARG A 367	15.108	-9.468	4.035	1.00	33.93	A	C
ATOM	34	NE	ARG A 367	13.776	-9.735	3.506	1.00	35.58	A	N
ATOM	35	CZ	ARG A 367	12.984	-10.722	3.911	1.00	36.40	A	C
ATOM	36	NH1	ARG A 367	13.391	-11.536	4.872	1.00	38.99	A	N
ATOM	37	NH2	ARG A 367	11.787	-10.893	3.357	1.00	32.22	A	N
ATOM	38	C	ARG A 367	17.404	-11.359	6.070	1.00	38.45	A	C
ATOM	39	O	ARG A 367	16.238	-11.716	6.214	1.00	38.19	A	O
ATOM	40	N	LYS A 368	18.409	-12.225	6.141	1.00	39.51	A	N
ATOM	41	CA	LYS A 368	18.066	-13.623	6.523	1.00	42.96	A	C
ATOM	42	CB	LYS A 368	19.134	-14.622	6.045	1.00	45.95	A	C
ATOM	43	CG	LYS A 368	20.210	-13.925	5.156	1.00	52.92	A	C
ATOM	44	CD	LYS A 368	20.880	-14.877	4.164	1.00	58.56	A	C
ATOM	45	CE	LYS A 368	20.962	-14.188	2.764	1.00	58.47	A	C
ATOM	46	NZ	LYS A 368	20.999	-15.273	1.734	1.00	56.55	A	N
ATOM	47	C	LYS A 368	17.869	-13.800	8.050	1.00	42.60	A	C
ATOM	48	O	LYS A 368	17.514	-14.862	8.545	1.00	43.45	A	O
ATOM	49	N	LEU A 369	18.138	-12.785	8.839	1.00	39.77	A	N
ATOM	50	CA	LEU A 369	17.766	-13.028	10.141	1.00	38.94	A	C
ATOM	51	CB	LEU A 369	18.860	-12.459	11.040	1.00	40.29	A	C
ATOM	52	CG	LEU A 369	20.150	-13.359	11.004	1.00	39.75	A	C
ATOM	53	CD1	LEU A 369	21.442	-12.708	11.586	1.00	40.73	A	C
ATOM	54	CD2	LEU A 369	19.887	-14.743	11.659	1.00	34.89	A	C
ATOM	55	C	LEU A 369	16.297	-12.487	10.308	1.00	38.09	A	C
ATOM	56	O	LEU A 369	15.807	-12.332	11.444	1.00	36.74	A	O
ATOM	57	N	LEU A 370	15.582	-12.281	9.179	1.00	35.52	A	N
ATOM	58	CA	LEU A 370	14.305	-11.624	9.243	1.00	34.99	A	C
ATOM	59	CB	LEU A 370	14.370	-10.146	8.711	1.00	34.65	A	C

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Figure 2A - 2

ATOM	60	CG	LEU A 370	13.131	-9.232	8.691	1.00	33.70	A	C
ATOM	61	CD1	LEU A 370	12.714	-8.608	10.196	1.00	29.78	A	C
ATOM	62	CD2	LEU A 370	13.122	-8.101	7.667	1.00	32.79	A	C
ATOM	63	C	LEU A 370	13.193	-12.312	8.601	1.00	35.10	A	C
ATOM	64	O	LEU A 370	13.320	-12.667	7.480	1.00	36.42	A	O
ATOM	65	N	THR A 371	12.011	-12.344	9.229	1.00	35.24	A	N
ATOM	66	CA	THR A 371	10.832	-13.004	8.661	1.00	34.98	A	C
ATOM	67	CB	THR A 371	10.568	-14.296	9.495	1.00	34.02	A	C
ATOM	68	OG1	THR A 371	11.783	-15.035	9.588	1.00	26.41	A	O
ATOM	69	CG2	THR A 371	9.524	-15.217	8.795	1.00	32.05	A	C
ATOM	70	C	THR A 371	9.609	-12.121	8.731	1.00	37.68	A	C
ATOM	71	O	THR A 371	9.272	-11.636	9.823	1.00	38.22	A	O
ATOM	72	N	LEU A 372	8.896	-11.976	7.618	1.00	39.64	A	N
ATOM	73	CA	LEU A 372	7.778	-11.058	7.594	1.00	43.53	A	C
ATOM	74	CB	LEU A 372	7.696	-10.178	6.331	1.00	43.08	A	C
ATOM	75	CG	LEU A 372	8.924	-9.299	6.109	1.00	45.40	A	C
ATOM	76	CD1	LEU A 372	8.985	-8.538	4.785	1.00	45.86	A	C
ATOM	77	CD2	LEU A 372	9.044	-8.335	7.327	1.00	47.51	A	C
ATOM	78	C	LEU A 372	6.630	-11.822	7.415	1.00	46.28	A	C
ATOM	79	O	LEU A 372	6.703	-12.808	6.737	1.00	45.18	A	O
ATOM	80	N	GLU A 373	5.514	-11.347	7.967	1.00	50.40	A	N
ATOM	81	CA	GLU A 373	4.268	-12.017	7.683	1.00	53.36	A	C
ATOM	82	C	GLU A 373	3.605	-11.444	6.410	1.00	54.57	A	C
ATOM	83	O	GLU A 373	4.310	-11.041	5.458	1.00	55.54	A	O
ATOM	84	CB	GLU A 373	3.330	-11.819	8.867	1.00	54.46	A	C
ATOM	85	CG	GLU A 373	3.783	-12.588	10.115	1.00	59.64	A	C
ATOM	86	CD	GLU A 373	2.768	-12.397	11.219	1.00	20.00	A	C
ATOM	87	OE1	GLU A 373	1.902	-11.545	11.078	1.00	20.00	A	O
ATOM	88	OE2	GLU A 373	2.855	-13.106	12.220	1.00	20.00	A	O
ATOM	88	N	ASP A 374	2.288	-11.462	6.367	1.00	55.94	A	N
ATOM	89	CA	ASP A 374	1.543	-11.139	5.155	1.00	57.56	A	C
ATOM	90	CB	ASP A 374	0.960	-12.440	4.512	1.00	57.44	A	C
ATOM	92	CG	ASP A 374	2.069	-13.422	3.989	0.50	56.72	A	C
ATOM	94	OD1	ASP A 374	3.204	-12.968	3.710	0.50	54.87	A	O
ATOM	96	OD2	ASP A 374	1.894	-14.667	3.812	0.50	55.66	A	O
ATOM	97	C	ASP A 374	0.448	-10.076	5.422	1.00	58.84	A	C
ATOM	98	O	ASP A 374	-0.029	-9.376	4.483	1.00	59.51	A	O
ATOM	99	N	LYS A 375	0.052	-9.999	6.700	1.00	59.50	A	N
ATOM	100	CA	LYS A 375	-0.956	-9.069	7.166	1.00	60.71	A	C
ATOM	101	CB	LYS A 375	-1.666	-9.573	8.431	1.00	61.45	A	C
ATOM	102	CG	LYS A 375	-2.749	-8.590	8.974	1.00	63.58	A	C
ATOM	103	CD	LYS A 375	-2.231	-7.758	10.159	1.00	66.11	A	C
ATOM	104	CE	LYS A 375	-3.392	-7.102	10.906	1.00	67.77	A	C
ATOM	105	NZ	LYS A 375	-2.976	-6.689	12.272	1.00	69.53	A	N
ATOM	106	C	LYS A 375	-0.296	-7.744	7.442	1.00	60.30	A	C
ATOM	107	O	LYS A 375	0.828	-7.679	7.904	1.00	60.39	A	O
ATOM	108	N	GLU A 376	-0.985	-6.670	7.153	1.00	60.16	A	N
ATOM	109	CA	GLU A 376	-0.345	-5.409	7.411	1.00	60.09	A	C
ATOM	110	CB	GLU A 376	-0.378	-4.536	6.148	1.00	60.70	A	C
ATOM	111	CG	GLU A 376	-1.722	-4.299	5.484	1.00	62.74	A	C
ATOM	112	CD	GLU A 376	-1.541	-3.421	4.224	1.00	66.19	A	C
ATOM	113	OE1	GLU A 376	-0.639	-3.753	3.390	1.00	68.04	A	O
ATOM	114	OE2	GLU A 376	-2.255	-2.390	4.072	1.00	66.15	A	O
ATOM	115	C	GLU A 376	-0.943	-4.724	8.619	1.00	58.87	A	C
ATOM	116	O	GLU A 376	-2.093	-4.951	8.910	1.00	59.43	A	O
ATOM	117	N	LEU A 377	-0.167	-3.875	9.282	1.00	57.55	A	N
ATOM	118	CA	LEU A 377	-0.589	-3.074	10.448	1.00	56.29	A	C
ATOM	119	CB	LEU A 377	0.578	-2.988	11.422	1.00	55.44	A	C
ATOM	120	CG	LEU A 377	1.128	-4.369	11.672	1.00	52.66	A	C
ATOM	121	CD1	LEU A 377	2.415	-4.386	12.476	1.00	51.67	A	C
ATOM	122	CD2	LEU A 377	-0.001	-5.100	12.397	1.00	51.50	A	C
ATOM	123	C	LEU A 377	-0.974	-1.664	10.046	1.00	56.42	A	C

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Figure 2A - 3

ATOM	124	O	LEU A 377	-2.030	-1.161	10.397	1.00	56.88	A	O
ATOM	125	N	GLY A 378	-0.097	-1.033	9.278	1.00	56.98	A	N
ATOM	126	CA	GLY A 378	-0.306	0.327	8.766	1.00	58.07	A	C
ATOM	127	C	GLY A 378	0.161	0.541	7.301	1.00	58.33	A	C
ATOM	128	O	GLY A 378	0.872	-0.332	6.704	1.00	57.34	A	O
ATOM	129	N	SER A 379	-0.236	1.687	6.730	1.00	58.58	A	N
ATOM	130	CA	SER A 379	0.061	1.990	5.335	1.00	60.21	A	C
ATOM	131	CB	SER A 379	-1.235	1.866	4.440	1.00	61.03	A	C
ATOM	132	OG	SER A 379	-2.262	0.961	4.954	1.00	61.85	A	O
ATOM	133	C	SER A 379	0.708	3.389	5.138	1.00	61.17	A	C
ATOM	134	O	SER A 379	0.125	4.437	5.529	1.00	61.65	A	O
ATOM	135	N	GLY A 380	1.892	3.455	4.534	1.00	61.37	A	N
ATOM	136	CA	GLY A 380	2.434	4.797	4.262	1.00	62.65	A	C
ATOM	137	C	GLY A 380	2.048	5.411	2.897	1.00	62.43	A	C
ATOM	138	O	GLY A 380	2.687	6.372	2.397	1.00	62.28	A	O
ATOM	139	N	GLY A 383	5.200	3.296	1.418	1.00	44.52	A	N
ATOM	140	CA	GLY A 383	4.347	2.097	1.484	1.00	44.44	A	C
ATOM	141	C	GLY A 383	3.590	1.649	2.748	1.00	44.18	A	C
ATOM	142	O	GLY A 383	2.878	2.424	3.473	1.00	46.06	A	O
ATOM	143	N	THR A 384	3.703	0.380	3.065	1.00	41.77	A	N
ATOM	144	CA	THR A 384	2.923	-0.143	4.192	1.00	40.57	A	C
ATOM	145	CB	THR A 384	2.529	-1.491	3.776	1.00	42.28	A	C
ATOM	146	OG1	THR A 384	2.826	-2.364	4.895	1.00	46.47	A	O
ATOM	147	CG2	THR A 384	3.575	-2.019	2.735	1.00	42.19	A	C
ATOM	148	C	THR A 384	3.756	-0.465	5.440	1.00	37.72	A	C
ATOM	149	O	THR A 384	4.938	-0.415	5.395	1.00	36.73	A	O
ATOM	150	N	VAL A 385	3.159	-0.989	6.491	1.00	35.77	A	N
ATOM	151	CA	VAL A 385	3.913	-1.426	7.661	1.00	34.47	A	C
ATOM	152	CB	VAL A 385	3.340	-0.772	8.864	1.00	34.63	A	C
ATOM	153	CG1	VAL A 385	4.058	-1.141	10.228	1.00	30.63	A	C
ATOM	154	CG2	VAL A 385	3.327	0.742	8.719	1.00	36.45	A	C
ATOM	155	C	VAL A 385	3.583	-2.893	7.875	1.00	35.96	A	C
ATOM	156	O	VAL A 385	2.409	-3.295	7.754	1.00	37.12	A	O
ATOM	157	N	LYS A 386	4.546	-3.734	8.231	1.00	34.81	A	N
ATOM	158	CA	LYS A 386	4.153	-5.086	8.495	1.00	35.88	A	C
ATOM	159	CB	LYS A 386	4.598	-6.003	7.360	1.00	36.63	A	C
ATOM	160	CG	LYS A 386	3.642	-5.980	6.167	1.00	41.51	A	C
ATOM	161	CD	LYS A 386	4.235	-6.751	4.970	1.00	49.64	A	C
ATOM	162	CE	LYS A 386	3.499	-6.546	3.540	1.00	54.70	A	C
ATOM	163	NZ	LYS A 386	2.603	-7.696	3.165	1.00	56.27	A	N
ATOM	164	C	LYS A 386	4.775	-5.599	9.787	1.00	35.77	A	C
ATOM	165	O	LYS A 386	5.774	-5.058	10.326	1.00	35.61	A	O
ATOM	166	N	LYS A 387	4.206	-6.704	10.233	1.00	35.48	A	N
ATOM	167	CA	LYS A 387	4.716	-7.407	11.362	1.00	36.07	A	C
ATOM	168	CB	LYS A 387	3.538	-7.865	12.242	1.00	36.59	A	C
ATOM	169	CG	LYS A 387	3.987	-8.521	13.532	1.00	37.45	A	C
ATOM	170	CD	LYS A 387	2.823	-9.467	14.099	1.00	42.24	A	C
ATOM	171	CE	LYS A 387	2.565	-9.205	15.631	1.00	41.23	A	C
ATOM	172	NZ	LYS A 387	1.601	-10.137	16.187	1.00	40.28	A	N
ATOM	173	C	LYS A 387	5.554	-8.600	10.955	1.00	34.68	A	C
ATOM	174	O	LYS A 387	5.330	-9.139	9.875	1.00	34.22	A	O
ATOM	175	N	GLY A 388	6.515	-8.958	11.832	1.00	34.01	A	N
ATOM	176	CA	GLY A 388	7.479	-10.049	11.683	1.00	34.44	A	C
ATOM	177	C	GLY A 388	8.480	-10.321	12.817	1.00	35.40	A	C
ATOM	178	O	GLY A 388	8.293	-9.854	14.001	1.00	36.13	A	O
ATOM	179	N	TYR A 389	9.557	-11.039	12.534	1.00	34.19	A	N
ATOM	180	CA	TYR A 389	10.475	-11.252	13.606	1.00	35.84	A	C
ATOM	181	CB	TYR A 389	10.225	-12.676	14.193	1.00	39.10	A	C
ATOM	182	CG	TYR A 389	8.744	-12.993	14.406	1.00	40.36	A	C
ATOM	183	CD1	TYR A 389	8.018	-13.415	13.411	1.00	40.90	A	C
ATOM	184	CE1	TYR A 389	6.702	-13.589	13.561	1.00	46.13	A	C
ATOM	185	CZ	TYR A 389	6.054	-13.344	14.741	1.00	46.61	A	C

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ATOM	186	OH	TYR	A	389	4.718	-13.599	14.730	1.00	52.06	A	O
ATOM	187	CE2	TYR	A	389	6.717	-12.871	15.793	1.00	43.52	A	C
ATOM	188	CD2	TYR	A	389	8.084	-12.687	15.640	1.00	43.48	A	C
ATOM	189	C	TYR	A	389	11.852	-11.208	13.090	1.00	36.54	A	C
ATOM	190	O	TYR	A	389	12.037	-11.368	11.917	1.00	38.04	A	O
ATOM	191	N	TYR	A	390	12.839	-11.027	13.954	1.00	37.14	A	N
ATOM	192	CA	TYR	A	390	14.224	-10.912	13.579	1.00	37.88	A	C
ATOM	193	CB	TYR	A	390	14.620	-9.445	13.540	1.00	36.55	A	C
ATOM	194	CG	TYR	A	390	16.002	-9.216	13.050	1.00	34.88	A	C
ATOM	195	CD1	TYR	A	390	16.249	-9.132	11.723	1.00	35.86	A	C
ATOM	196	CE1	TYR	A	390	17.530	-8.920	11.198	1.00	33.48	A	C
ATOM	197	CZ	TYR	A	390	18.589	-8.754	11.974	1.00	35.80	A	C
ATOM	198	OH	TYR	A	390	19.882	-8.496	11.338	1.00	38.24	A	O
ATOM	199	CE2	TYR	A	390	18.403	-8.805	13.386	1.00	34.00	A	C
ATOM	200	CD2	TYR	A	390	17.082	-9.034	13.916	1.00	35.70	A	C
ATOM	201	C	TYR	A	390	15.094	-11.612	14.631	1.00	39.84	A	C
ATOM	202	O	TYR	A	390	14.934	-11.314	15.793	1.00	39.46	A	O
ATOM	203	N	GLN	A	391	16.021	-12.484	14.215	1.00	41.67	A	N
ATOM	204	CA	GLN	A	391	16.837	-13.223	15.103	1.00	44.97	A	C
ATOM	205	CB	GLN	A	391	17.261	-14.668	14.621	1.00	46.33	A	C
ATOM	206	CG	GLN	A	391	17.846	-15.608	15.807	1.00	48.09	A	C
ATOM	207	CD	GLN	A	391	18.651	-16.968	15.363	1.00	51.81	A	C
ATOM	208	OE1	GLN	A	391	18.718	-17.363	14.173	1.00	50.20	A	O
ATOM	209	NE2	GLN	A	391	19.238	-17.650	16.369	1.00	52.81	A	N
ATOM	210	C	GLN	A	391	18.060	-12.512	15.421	1.00	46.62	A	C
ATOM	211	O	GLN	A	391	19.100	-12.660	14.760	1.00	46.60	A	O
ATOM	212	N	MET	A	392	17.973	-11.828	16.530	1.00	48.67	A	N
ATOM	213	CA	MET	A	392	19.140	-11.211	17.075	1.00	52.04	A	C
ATOM	214	CB	MET	A	392	18.686	-10.043	17.897	1.00	53.60	A	C
ATOM	215	CG	MET	A	392	17.273	-10.259	18.286	1.00	54.57	A	C
ATOM	216	SD	MET	A	392	16.688	-8.751	17.798	1.00	60.27	A	S
ATOM	217	CE	MET	A	392	17.847	-7.622	18.750	1.00	61.58	A	C
ATOM	218	C	MET	A	392	19.801	-12.366	17.876	1.00	52.19	A	C
ATOM	219	O	MET	A	392	19.154	-13.229	18.419	1.00	53.40	A	O
ATOM	220	N	LYS	A	393	21.103	-12.419	17.846	1.00	52.34	A	N
ATOM	221	CA	LYS	A	393	21.794	-13.624	18.304	1.00	53.42	A	C
ATOM	222	CB	LYS	A	393	22.551	-13.352	19.588	1.00	52.97	A	C
ATOM	223	CG	LYS	A	393	23.165	-11.973	19.503	1.00	54.62	A	C
ATOM	224	CD	LYS	A	393	23.647	-11.576	20.863	1.00	56.60	A	C
ATOM	225	CE	LYS	A	393	24.421	-10.259	20.850	1.00	58.50	A	C
ATOM	226	NZ	LYS	A	393	25.976	-10.439	20.823	1.00	54.96	A	N
ATOM	227	C	LYS	A	393	20.945	-14.872	18.438	1.00	53.42	A	C
ATOM	228	O	LYS	A	393	20.801	-15.585	17.446	1.00	54.25	A	O
ATOM	229	N	LYS	A	394	20.478	-15.167	19.665	1.00	52.85	A	N
ATOM	230	CA	LYS	A	394	19.613	-16.298	19.944	1.00	51.47	A	C
ATOM	231	CB	LYS	A	394	19.781	-16.882	21.349	1.00	53.24	A	C
ATOM	232	CG	LYS	A	394	19.268	-18.366	21.482	1.00	54.88	A	C
ATOM	233	CD	LYS	A	394	18.506	-18.680	22.741	1.00	57.49	A	C
ATOM	234	CE	LYS	A	394	18.694	-17.614	23.753	1.00	59.08	A	C
ATOM	235	NZ	LYS	A	394	20.018	-17.794	24.352	1.00	59.70	A	N
ATOM	236	C	LYS	A	394	18.226	-15.834	19.910	1.00	50.65	A	C
ATOM	237	O	LYS	A	394	17.521	-16.077	18.931	1.00	51.86	A	O
ATOM	238	N	VAL	A	395	17.786	-15.199	20.989	1.00	48.35	A	N
ATOM	239	CA	VAL	A	395	16.345	-14.827	21.113	1.00	46.49	A	C
ATOM	240	CB	VAL	A	395	16.209	-13.822	22.250	1.00	47.05	A	C
ATOM	241	CG1	VAL	A	395	17.640	-13.217	22.578	1.00	49.72	A	C
ATOM	242	CG2	VAL	A	395	15.224	-12.772	21.966	1.00	45.64	A	C
ATOM	243	C	VAL	A	395	15.722	-14.225	19.855	1.00	43.67	A	C
ATOM	244	O	VAL	A	395	16.388	-13.587	19.071	1.00	44.16	A	O
ATOM	245	N	VAL	A	396	14.443	-14.411	19.695	1.00	40.06	A	N
ATOM	246	CA	VAL	A	396	13.672	-13.879	18.630	1.00	38.09	A	C
ATOM	247	CB	VAL	A	396	12.900	-14.941	18.020	1.00	38.18	A	C

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ATOM	248	CG1	VAL	A	396	11.868	-14.406	16.967	1.00	37.67	A	C
ATOM	249	CG2	VAL	A	396	13.878	-15.849	17.364	1.00	39.56	A	C
ATOM	250	C	VAL	A	396	12.721	-12.779	19.091	1.00	37.73	A	C
ATOM	251	O	VAL	A	396	12.100	-12.860	20.122	1.00	35.70	A	O
ATOM	252	N	LYS	A	397	12.574	-11.754	18.241	1.00	37.21	A	N
ATOM	253	CA	LYS	A	397	11.938	-10.501	18.660	1.00	34.98	A	C
ATOM	254	CB	LYS	A	397	13.042	-9.429	18.737	1.00	34.72	A	C
ATOM	255	CG	LYS	A	397	13.063	-8.503	19.959	1.00	37.88	A	C
ATOM	256	CD	LYS	A	397	12.673	-7.043	19.612	1.00	38.43	A	C
ATOM	257	CE	LYS	A	397	13.083	-5.996	20.645	1.00	36.88	A	C
ATOM	258	NZ	LYS	A	397	12.709	-6.192	22.051	1.00	36.08	A	N
ATOM	259	C	LYS	A	397	10.867	-10.187	17.621	1.00	33.00	A	C
ATOM	260	O	LYS	A	397	11.151	-10.325	16.400	1.00	32.23	A	O
ATOM	261	N	THR	A	398	9.630	-9.906	18.054	1.00	29.02	A	N
ATOM	262	CA	THR	A	398	8.705	-9.501	17.058	1.00	28.97	A	C
ATOM	263	CB	THR	A	398	7.300	-9.782	17.423	1.00	30.35	A	C
ATOM	264	OG1	THR	A	398	6.754	-8.608	17.914	1.00	35.99	A	O
ATOM	265	CG2	THR	A	398	7.201	-10.739	18.604	1.00	30.78	A	C
ATOM	266	C	THR	A	398	8.919	-8.047	16.689	1.00	27.39	A	C
ATOM	267	O	THR	A	398	9.374	-7.276	17.511	1.00	24.90	A	O
ATOM	268	N	VAL	A	399	8.647	-7.654	15.445	1.00	26.29	A	N
ATOM	269	CA	VAL	A	399	8.951	-6.323	15.192	1.00	27.57	A	C
ATOM	270	CB	VAL	A	399	10.353	-6.199	14.489	1.00	29.01	A	C
ATOM	271	CG1	VAL	A	399	11.541	-6.477	15.406	1.00	24.62	A	C
ATOM	272	CG2	VAL	A	399	10.379	-7.070	13.261	1.00	31.07	A	C
ATOM	273	C	VAL	A	399	7.959	-5.817	14.262	1.00	28.71	A	C
ATOM	274	O	VAL	A	399	7.218	-6.552	13.695	1.00	29.28	A	O
ATOM	275	N	ALA	A	400	7.943	-4.509	14.078	1.00	29.56	A	N
ATOM	276	CA	ALA	A	400	7.113	-3.881	13.056	1.00	28.94	A	C
ATOM	277	CB	ALA	A	400	6.275	-2.765	13.639	1.00	27.99	A	C
ATOM	278	C	ALA	A	400	8.070	-3.311	12.031	1.00	28.51	A	C
ATOM	279	O	ALA	A	400	9.171	-2.893	12.385	1.00	27.38	A	O
ATOM	280	N	VAL	A	401	7.633	-3.207	10.789	1.00	28.10	A	N
ATOM	281	CA	VAL	A	401	8.622	-2.943	9.783	1.00	29.29	A	C
ATOM	282	CB	VAL	A	401	8.968	-4.250	9.034	1.00	29.82	A	C
ATOM	283	CG1	VAL	A	401	9.980	-3.956	7.890	1.00	29.61	A	C
ATOM	284	CG2	VAL	A	401	9.505	-5.400	9.988	1.00	26.24	A	C
ATOM	285	C	VAL	A	401	8.005	-2.027	8.779	1.00	31.86	A	C
ATOM	286	O	VAL	A	401	6.933	-2.390	8.189	1.00	30.62	A	O
ATOM	287	N	LYS	A	402	8.599	-0.830	8.596	1.00	33.32	A	N
ATOM	288	CA	LYS	A	402	7.987	0.103	7.662	1.00	37.07	A	C
ATOM	289	CB	LYS	A	402	8.423	1.543	7.976	1.00	37.20	A	C
ATOM	290	CG	ALYS	A	402	7.681	2.169	9.086	0.80	37.79	A	C
ATOM	291	CG	BLYS	A	402	7.505	2.670	7.409	0.20	36.13	A	C
ATOM	292	CD	ALYS	A	402	7.903	3.621	9.120	0.80	35.67	A	C
ATOM	293	CD	BLYS	A	402	6.564	2.200	6.294	0.20	34.98	A	C
ATOM	294	CE	ALYS	A	402	6.757	4.322	9.905	0.80	36.08	A	C
ATOM	295	CE	BLYS	A	402	6.441	3.193	5.111	0.20	34.21	A	C
ATOM	296	NZ	ALYS	A	402	7.075	5.782	10.169	0.80	36.80	A	N
ATOM	297	NZ	BLYS	A	402	6.026	4.626	5.425	0.20	33.00	A	N
ATOM	298	C	LYS	A	402	8.630	-0.295	6.370	1.00	38.76	A	C
ATOM	299	O	LYS	A	402	9.879	-0.332	6.288	1.00	40.93	A	O
ATOM	300	N	ILE	A	403	7.866	-0.593	5.357	1.00	39.23	A	N
ATOM	301	CA	ILE	A	403	8.520	-0.987	4.125	1.00	42.30	A	C
ATOM	302	CB	ILE	A	403	7.944	-2.334	3.765	1.00	42.42	A	C
ATOM	303	CG1	ILE	A	403	8.260	-3.402	4.806	1.00	41.06	A	C
ATOM	304	CD1	ILE	A	403	7.818	-4.677	4.240	1.00	36.86	A	C
ATOM	305	CG2	ILE	A	403	8.415	-2.793	2.391	1.00	42.03	A	C
ATOM	306	C	ILE	A	403	8.237	-0.130	2.931	1.00	44.24	A	C
ATOM	307	O	ILE	A	403	7.220	0.422	2.859	1.00	45.87	A	O
ATOM	308	N	LEU	A	404	9.034	-0.139	1.886	1.00	47.73	A	N
ATOM	309	CA	LEU	A	404	8.678	0.622	0.612	1.00	49.02	A	C

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ATOM	310	CB	LEU	A	404	9.939	1.055	-0.052	1.00	48.85	A	C
ATOM	311	CG	LEU	A	404	10.549	2.069	0.896	1.00	48.03	A	C
ATOM	312	CD1	LEU	A	404	12.006	2.274	0.503	1.00	50.43	A	C
ATOM	313	CD2	LEU	A	404	9.787	3.366	0.809	1.00	48.17	A	C
ATOM	314	C	LEU	A	404	7.814	0.050	-0.515	1.00	50.29	A	C
ATOM	315	O	LEU	A	404	7.477	0.778	-1.494	1.00	51.27	A	O
ATOM	316	N	ALA	A	412	10.209	10.017	-5.151	1.00	58.13	A	N
ATOM	317	CA	ALA	A	412	11.419	9.297	-4.732	1.00	57.61	A	C
ATOM	318	CB	ALA	A	412	12.542	9.477	-5.766	1.00	57.79	A	C
ATOM	319	C	ALA	A	412	11.863	9.685	-3.302	1.00	57.24	A	C
ATOM	320	O	ALA	A	412	12.787	10.489	-3.084	1.00	56.86	A	O
ATOM	321	N	LEU	A	413	11.147	9.140	-2.306	1.00	57.21	A	N
ATOM	322	CA	LEU	A	413	11.386	9.510	-0.875	1.00	56.11	A	C
ATOM	323	CB	LEU	A	413	10.140	10.153	-0.303	1.00	56.55	A	C
ATOM	324	CG	LEU	A	413	8.968	9.138	-0.206	1.00	59.34	A	C
ATOM	325	CD1	LEU	A	413	8.014	9.028	-1.445	1.00	61.00	A	C
ATOM	326	CD2	LEU	A	413	9.537	7.773	0.107	1.00	58.16	A	C
ATOM	327	C	LEU	A	413	11.958	8.408	0.093	1.00	54.76	A	C
ATOM	328	O	LEU	A	413	11.444	8.122	1.214	1.00	54.34	A	O
ATOM	329	N	LYS	A	414	13.044	7.804	-0.358	1.00	52.38	A	N
ATOM	330	CA	LYS	A	414	13.855	6.995	0.491	1.00	50.17	A	C
ATOM	331	CB	LYS	A	414	15.026	6.407	-0.311	1.00	50.89	A	C
ATOM	332	CG	LYS	A	414	15.780	5.278	0.404	1.00	52.10	A	C
ATOM	333	CD	LYS	A	414	16.929	4.651	-0.429	1.00	53.70	A	C
ATOM	334	CE	LYS	A	414	17.963	3.923	0.464	1.00	53.89	A	C
ATOM	335	NZ	LYS	A	414	18.714	2.779	-0.216	1.00	52.24	A	N
ATOM	336	C	LYS	A	414	14.429	7.926	1.531	1.00	48.19	A	C
ATOM	337	O	LYS	A	414	14.942	7.472	2.554	1.00	47.11	A	O
ATOM	338	N	ASP	A	415	14.356	9.231	1.290	1.00	45.65	A	N
ATOM	339	CA	ASP	A	415	15.053	10.107	2.209	1.00	45.21	A	C
ATOM	340	CB	ASP	A	415	15.378	11.368	1.505	1.00	45.76	A	C
ATOM	341	CG	AASP	A	415	16.547	11.232	0.493	0.30	45.52	A	C
ATOM	342	CG	BASP	A	415	14.175	11.964	0.938	0.70	46.36	A	C
ATOM	343	OD1AASP	A	415	17.693	10.886	0.864	0.30	44.27	A	O	
ATOM	344	OD1BASP	A	415	13.111	11.244	0.975	0.70	47.51	A	O	
ATOM	345	OD2AASP	A	415	16.402	11.495	-0.716	0.30	46.89	A	O	
ATOM	346	OD2BASP	A	415	14.207	13.122	0.479	0.70	45.87	A	O	
ATOM	347	C	ASP	A	415	14.248	10.454	3.473	1.00	43.79	A	C
ATOM	348	O	ASP	A	415	14.788	10.688	4.526	1.00	44.11	A	O
ATOM	349	N	GLU	A	416	12.961	10.508	3.377	1.00	42.41	A	N
ATOM	350	CA	GLU	A	416	12.250	10.783	4.587	1.00	43.04	A	C
ATOM	351	CB	GLU	A	416	10.794	10.852	4.204	1.00	43.82	A	C
ATOM	352	CG	AGLU	A	416	10.407	12.176	3.619	0.50	44.48	A	C
ATOM	353	CG	BGLU	A	416	9.774	11.049	5.321	0.50	45.37	A	C
ATOM	354	CD	AGLU	A	416	10.426	12.110	2.119	0.50	45.55	A	C
ATOM	355	CD	BGLU	A	416	8.403	11.479	4.786	0.50	45.17	A	C
ATOM	356	OE1AGLU	A	416	11.167	11.217	1.603	0.50	44.89	A	O	
ATOM	357	OE1BGLU	A	416	8.087	11.240	3.590	0.50	45.44	A	O	
ATOM	358	OE2AGLU	A	416	9.713	12.949	1.492	0.50	44.69	A	O	
ATOM	359	OE2BGLU	A	416	7.647	12.065	5.568	0.50	44.05	A	O	
ATOM	360	C	GLU	A	416	12.533	9.649	5.595	1.00	42.27	A	C
ATOM	361	O	GLU	A	416	13.028	9.852	6.720	1.00	41.84	A	O
ATOM	362	N	LEU	A	417	12.294	8.435	5.131	1.00	40.79	A	N
ATOM	363	CA	LEU	A	417	12.473	7.279	5.912	1.00	40.48	A	C
ATOM	364	CB	LEU	A	417	12.522	6.123	4.997	1.00	39.86	A	C
ATOM	365	CG	LEU	A	417	11.675	5.045	5.571	1.00	43.22	A	C
ATOM	366	CD1	LEU	A	417	10.285	4.866	4.803	1.00	44.67	A	C
ATOM	367	CD2	LEU	A	417	12.614	3.814	5.523	1.00	43.65	A	C
ATOM	368	C	LEU	A	417	13.837	7.331	6.512	1.00	41.30	A	C
ATOM	369	O	LEU	A	417	14.016	7.009	7.758	1.00	39.72	A	O
ATOM	370	N	LEU	A	418	14.808	7.711	5.634	1.00	40.66	A	N
ATOM	371	CA	LEU	A	418	16.189	7.655	6.060	1.00	40.70	A	N

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## Figure 2A - 7

ATOM	372	CB	LEU A 418	17.143	7.973	4.994	1.00	42.35	A	C
ATOM	373	CG	LEU A 418	17.689	6.667	4.462	1.00	47.12	A	C
ATOM	374	CD1	LEU A 418	18.186	6.946	3.020	1.00	51.50	A	C
ATOM	375	CD2	LEU A 418	18.802	6.101	5.354	1.00	49.27	A	C
ATOM	376	C	LEU A 418	16.432	8.560	7.198	1.00	39.86	A	C
ATOM	377	O	LEU A 418	17.137	8.200	8.162	1.00	37.00	A	O
ATOM	378	N	ALA A 419	15.773	9.713	7.149	1.00	39.67	A	N
ATOM	379	CA	ALA A 419	16.042	10.690	8.187	1.00	39.56	A	C
ATOM	380	CB	ALA A 419	15.613	12.076	7.725	1.00	39.95	A	C
ATOM	381	C	ALA A 419	15.426	10.233	9.501	1.00	39.38	A	C
ATOM	382	O	ALA A 419	16.036	10.294	10.643	1.00	39.53	A	O
ATOM	383	N	GLU A 420	14.280	9.604	9.303	1.00	37.99	A	N
ATOM	384	CA	GLU A 420	13.566	9.073	10.419	1.00	37.77	A	C
ATOM	385	CB	GLU A 420	12.389	8.333	9.835	1.00	38.02	A	C
ATOM	386	CG	AGLU A 420	11.769	7.383	10.865	0.30	35.88	A	C
ATOM	387	CG	BGLU A 420	11.116	8.160	10.566	0.70	37.66	A	C
ATOM	388	CD	AGLU A 420	10.240	7.452	10.961	0.30	34.78	A	C
ATOM	389	CD	BGLU A 420	9.976	7.839	9.619	0.70	38.25	A	C
ATOM	390	OE1	AGLU A 420	9.625	7.976	9.984	0.30	33.95	A	O
ATOM	391	OE1	BGLU A 420	9.757	8.590	8.662	0.70	40.19	A	O
ATOM	392	OE2	AGLU A 420	9.669	6.988	12.028	0.30	30.48	A	O
ATOM	393	OE2	BGLU A 420	9.273	6.840	9.833	0.70	38.27	A	O
ATOM	394	C	GLU A 420	14.494	8.091	11.186	1.00	37.92	A	C
ATOM	395	O	GLU A 420	14.729	8.242	12.420	1.00	36.96	A	O
ATOM	396	N	ALA A 421	15.032	7.105	10.452	1.00	36.34	A	N
ATOM	397	CA	ALA A 421	15.975	6.156	11.010	1.00	35.30	A	C
ATOM	398	CB	ALA A 421	16.443	5.206	9.912	1.00	35.46	A	C
ATOM	399	C	ALA A 421	17.170	6.849	11.643	1.00	34.65	A	C
ATOM	400	O	ALA A 421	17.689	6.467	12.726	1.00	31.31	A	O
ATOM	401	N	ASN A 422	17.555	7.935	10.998	1.00	35.59	A	N
ATOM	402	CA	ASN A 422	18.682	8.662	11.509	1.00	39.03	A	C
ATOM	403	CB	ASN A 422	19.349	9.561	10.415	1.00	42.24	A	C
ATOM	404	CG	ASN A 422	20.287	8.722	9.340	1.00	49.17	A	C
ATOM	405	OD1	ASN A 422	20.892	7.622	9.638	1.00	53.39	A	O
ATOM	406	ND2	ASN A 422	20.383	9.283	8.101	1.00	52.05	A	N
ATOM	407	C	ASN A 422	18.350	9.405	12.846	1.00	38.97	A	C
ATOM	408	O	ASN A 422	19.216	9.727	13.633	1.00	39.72	A	O
ATOM	409	N	VAL A 423	17.102	9.680	13.121	1.00	37.54	A	N
ATOM	410	CA	VAL A 423	16.839	10.149	14.409	1.00	36.57	A	C
ATOM	411	CB	VAL A 423	15.596	10.830	14.297	1.00	38.14	A	C
ATOM	412	CG1	VAL A 423	15.037	11.181	15.658	1.00	39.28	A	C
ATOM	413	CG2	VAL A 423	15.757	11.972	13.326	1.00	37.95	A	C
ATOM	414	C	VAL A 423	16.643	9.040	15.430	1.00	35.56	A	C
ATOM	415	O	VAL A 423	17.070	9.091	16.642	1.00	32.89	A	O
ATOM	416	N	MET A 424	16.024	7.985	14.963	1.00	35.60	A	N
ATOM	417	CA	MET A 424	15.697	6.931	15.939	1.00	36.32	A	C
ATOM	418	CB	MET A 424	14.700	5.886	15.432	1.00	36.49	A	C
ATOM	419	CG	MET A 424	13.406	6.441	14.699	1.00	38.22	A	C
ATOM	420	SD	MET A 424	12.208	5.053	14.299	1.00	40.02	A	S
ATOM	421	CE	MET A 424	11.948	4.515	16.110	1.00	31.95	A	C
ATOM	422	C	MET A 424	17.006	6.338	16.326	1.00	36.31	A	C
ATOM	423	O	MET A 424	17.273	6.033	17.493	1.00	35.89	A	O
ATOM	424	N	GLN A 425	17.882	6.301	15.358	1.00	36.82	A	N
ATOM	425	CA	GLN A 425	19.154	5.757	15.634	1.00	38.18	A	C
ATOM	426	CB	GLN A 425	20.005	5.824	14.422	1.00	39.45	A	C
ATOM	427	CG	GLN A 425	21.097	4.854	14.447	1.00	46.21	A	C
ATOM	428	CD	GLN A 425	22.346	5.634	14.449	1.00	53.70	A	C
ATOM	429	OE1	GLN A 425	22.269	6.881	14.562	1.00	57.17	A	O
ATOM	430	NE2	GLN A 425	23.509	4.957	14.352	1.00	53.97	A	N
ATOM	431	C	GLN A 425	19.833	6.439	16.789	1.00	38.39	A	C
ATOM	432	O	GLN A 425	20.592	5.745	17.498	1.00	38.06	A	O
ATOM	433	N	GLN A 426	19.578	7.755	17.003	1.00	36.53	A	N

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Figure 2A - 8

ATOM	434	CA	GLN	A	426	20.265	8.475	18.075	1.00	35.44	A	C
ATOM	435	CB	GLN	A	426	20.544	9.985	17.718	1.00	36.40	A	C
ATOM	436	CG	GLN	A	426	21.150	10.253	16.304	1.00	38.67	A	C
ATOM	437	CD	GLN	A	426	21.079	11.744	15.757	1.00	40.71	A	C
ATOM	438	OE1	GLN	A	426	21.736	12.624	16.348	1.00	47.82	A	O
ATOM	439	NE2	GLN	A	426	20.278	12.022	14.654	1.00	30.22	A	N
ATOM	440	C	GLN	A	426	19.491	8.453	19.409	1.00	33.75	A	C
ATOM	441	O	GLN	A	426	19.903	9.058	20.325	1.00	32.52	A	O
ATOM	442	N	LEU	A	427	18.360	7.777	19.504	1.00	32.05	A	N
ATOM	443	CA	LEU	A	427	17.579	7.857	20.717	1.00	29.95	A	C
ATOM	444	CB	LEU	A	427	16.091	8.227	20.379	1.00	29.61	A	C
ATOM	445	CG	LEU	A	427	15.900	9.530	19.538	1.00	29.80	A	C
ATOM	446	CD1	LEU	A	427	14.528	9.808	18.940	1.00	27.34	A	C
ATOM	447	CD2	LEU	A	427	16.451	10.840	20.342	1.00	28.72	A	C
ATOM	448	C	LEU	A	427	17.533	6.593	21.500	1.00	29.64	A	C
ATOM	449	O	LEU	A	427	17.466	5.490	20.960	1.00	26.21	A	O
ATOM	450	N	ASP	A	428	17.416	6.756	22.810	1.00	30.30	A	N
ATOM	451	CA	ASP	A	428	17.234	5.600	23.580	1.00	31.05	A	C
ATOM	452	CB	ASP	A	428	18.647	5.016	23.728	1.00	33.51	A	C
ATOM	453	CG	ASP	A	428	18.700	3.924	24.720	1.00	37.31	A	C
ATOM	454	OD1	ASP	A	428	18.113	2.841	24.415	1.00	37.00	A	O
ATOM	455	OD2	ASP	A	428	19.289	4.115	25.843	1.00	40.95	A	O
ATOM	456	C	ASP	A	428	16.581	5.868	24.938	1.00	30.50	A	C
ATOM	457	O	ASP	A	428	17.239	6.361	25.945	1.00	27.35	A	O
ATOM	458	N	ASN	A	429	15.310	5.434	25.010	1.00	29.43	A	N
ATOM	459	CA	ASN	A	429	14.483	5.694	26.194	1.00	28.28	A	C
ATOM	460	CB	ASN	A	429	14.004	7.144	26.156	1.00	28.23	A	C
ATOM	461	CG	ASN	A	429	12.894	7.446	27.110	1.00	28.84	A	C
ATOM	462	OD1	ASN	A	429	11.719	7.382	26.737	1.00	27.02	A	O
ATOM	463	ND2	ASN	A	429	13.242	7.912	28.303	1.00	29.51	A	N
ATOM	464	C	ASN	A	429	13.350	4.754	26.142	1.00	28.09	A	C
ATOM	465	O	ASN	A	429	12.879	4.385	25.104	1.00	27.03	A	O
ATOM	466	N	PRO	A	430	12.919	4.343	27.295	1.00	28.08	A	N
ATOM	467	CA	PRO	A	430	11.827	3.407	27.368	1.00	28.50	A	C
ATOM	468	CB	PRO	A	430	11.680	3.113	28.852	1.00	30.10	A	C
ATOM	469	CG	PRO	A	430	13.049	3.485	29.375	1.00	29.22	A	C
ATOM	470	CD	PRO	A	430	13.465	4.714	28.593	1.00	28.30	A	C
ATOM	471	C	PRO	A	430	10.564	4.011	26.855	1.00	28.14	A	C
ATOM	472	O	PRO	A	430	9.650	3.221	26.571	1.00	27.56	A	O
ATOM	473	N	TYR	A	431	10.430	5.313	26.694	1.00	26.55	A	N
ATOM	474	CA	TYR	A	431	9.108	5.702	26.169	1.00	25.30	A	C
ATOM	475	CB	TYR	A	431	8.540	6.715	27.043	1.00	23.86	A	C
ATOM	476	CG	TYR	A	431	8.506	6.153	28.378	1.00	24.84	A	C
ATOM	477	CD1	TYR	A	431	9.453	6.437	29.281	1.00	25.44	A	C
ATOM	478	CE1	TYR	A	431	9.374	5.898	30.556	1.00	28.90	A	C
ATOM	479	CZ	TYR	A	431	8.423	4.977	30.825	1.00	31.11	A	C
ATOM	480	OH	TYR	A	431	8.359	4.386	32.050	1.00	37.30	A	O
ATOM	481	CE2	TYR	A	431	7.531	4.609	29.891	1.00	28.41	A	C
ATOM	482	CD2	TYR	A	431	7.558	5.188	28.709	1.00	26.75	A	C
ATOM	483	C	TYR	A	431	9.144	6.120	24.722	1.00	24.70	A	C
ATOM	484	O	TYR	A	431	8.273	6.784	24.256	1.00	23.28	A	O
ATOM	485	N	ILE	A	432	10.123	5.609	24.006	1.00	24.57	A	N
ATOM	486	CA	ILE	A	432	10.252	5.951	22.608	1.00	25.70	A	C
ATOM	487	CB	ILE	A	432	11.486	6.633	22.503	1.00	27.66	A	C
ATOM	488	CG1	ILE	A	432	11.529	7.733	23.592	1.00	29.07	A	C
ATOM	489	CD1	ILE	A	432	10.654	8.851	23.222	1.00	28.16	A	C
ATOM	490	CG2	ILE	A	432	11.713	7.151	21.032	1.00	28.15	A	C
ATOM	491	C	ILE	A	432	10.349	4.720	21.775	1.00	23.96	A	C
ATOM	492	O	ILE	A	432	11.126	3.885	22.053	1.00	19.28	A	O
ATOM	493	N	VAL	A	433	9.523	4.562	20.757	1.00	25.04	A	N
ATOM	494	CA	VAL	A	433	9.732	3.418	19.867	1.00	26.29	A	C
ATOM	495	CB	VAL	A	433	8.889	3.481	18.578	1.00	25.85	A	C



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Figure 2A - 9

ATOM	496	CG1	VAL	A	433	9.342	2.447	17.537	1.00	27.90	A	C
ATOM	497	CG2	VAL	A	433	7.481	3.129	18.871	1.00	23.88	A	C
ATOM	498	C	VAL	A	433	11.236	3.300	19.497	1.00	26.33	A	C
ATOM	499	O	VAL	A	433	11.755	4.171	19.051	1.00	26.13	A	O
ATOM	500	N	ARG	A	434	11.891	2.191	19.730	1.00	27.43	A	N
ATOM	501	CA	ARG	A	434	13.217	1.941	19.313	1.00	30.12	A	C
ATOM	502	CB	ARG	A	434	13.847	0.956	20.313	1.00	31.08	A	C
ATOM	503	CG	AARG	A	434	13.141	0.791	21.613	0.70	30.03	A	C
ATOM	504	CG	BARG	A	434	14.087	1.610	21.683	0.30	32.71	A	C
ATOM	505	CD	AARG	A	434	13.934	0.070	22.668	0.70	30.61	A	C
ATOM	506	CD	BARG	A	434	12.843	2.175	22.432	0.30	34.76	A	C
ATOM	507	NE	AARG	A	434	14.712	0.922	23.594	0.70	32.24	A	N
ATOM	508	NE	BARG	A	434	12.360	1.275	23.485	0.30	36.36	A	N
ATOM	509	CZ	AARG	A	434	15.678	1.800	23.268	0.70	34.10	A	C
ATOM	510	CZ	BARG	A	434	13.160	0.649	24.345	0.30	37.59	A	C
ATOM	511	NH1AARG	A	434	15.998	2.045	21.998	0.70	36.90	A	N	
ATOM	512	NH1BARG	A	434	14.463	0.881	24.311	0.30	38.40	A	N	
ATOM	513	NH2AARG	A	434	16.300	2.483	24.221	0.70	33.07	A	N	
ATOM	514	NH2BARG	A	434	12.671	-0.204	25.245	0.30	37.43	A	N	
ATOM	515	C	ARG	A	434	13.296	1.263	17.931	1.00	30.97	A	C
ATOM	516	O	ARG	A	434	12.476	0.485	17.610	1.00	31.54	A	O
ATOM	517	N	MET	A	435	14.302	1.593	17.130	1.00	32.62	A	N
ATOM	518	CA	MET	A	435	14.510	0.970	15.812	1.00	34.36	A	C
ATOM	519	CB	MET	A	435	14.923	2.014	14.725	1.00	34.31	A	C
ATOM	520	CG	MET	A	435	16.412	2.218	14.585	1.00	37.70	A	C
ATOM	521	SD	MET	A	435	16.896	2.867	12.857	1.00	41.81	A	S
ATOM	522	CE	MET	A	435	15.436	2.154	12.084	1.00	39.11	A	C
ATOM	523	C	MET	A	435	15.503	-0.230	15.863	1.00	33.88	A	C
ATOM	524	O	MET	A	435	16.587	-0.151	16.449	1.00	32.94	A	O
ATOM	525	N	ILE	A	436	15.120	-1.379	15.334	1.00	33.52	A	N
ATOM	526	CA	ILE	A	436	16.073	-2.458	15.445	1.00	34.43	A	C
ATOM	527	CB	ILE	A	436	15.396	-3.788	15.214	1.00	34.01	A	C
ATOM	528	CG1	ILE	A	436	14.215	-3.937	16.158	1.00	32.63	A	C
ATOM	529	CD1	ILE	A	436	14.614	-3.694	17.724	1.00	31.40	A	C
ATOM	530	CG2	ILE	A	436	16.408	-4.886	15.541	1.00	35.64	A	C
ATOM	531	C	ILE	A	436	17.178	-2.160	14.351	1.00	35.01	A	C
ATOM	532	O	ILE	A	436	18.370	-2.161	14.644	1.00	35.07	A	O
ATOM	533	N	GLY	A	437	16.767	-1.888	13.115	1.00	32.83	A	N
ATOM	534	CA	GLY	A	437	17.742	-1.460	12.168	1.00	31.93	A	C
ATOM	535	C	GLY	A	437	17.076	-1.162	10.901	1.00	32.20	A	C
ATOM	536	O	GLY	A	437	15.873	-0.953	10.821	1.00	31.27	A	O
ATOM	537	N	ILE	A	438	17.844	-1.177	9.842	1.00	34.48	A	N
ATOM	538	CA	ILE	A	438	17.214	-0.957	8.499	1.00	35.88	A	C
ATOM	539	CB	ILE	A	438	17.809	0.250	7.766	1.00	36.48	A	C
ATOM	540	CG1	ILE	A	438	19.310	0.161	7.780	1.00	38.05	A	C
ATOM	541	CD1	ILE	A	438	19.871	1.565	8.177	1.00	45.07	A	C
ATOM	542	CG2	ILE	A	438	17.500	1.603	8.458	1.00	32.69	A	C
ATOM	543	C	ILE	A	438	17.692	-2.141	7.813	1.00	36.81	A	C
ATOM	544	O	ILE	A	438	18.764	-2.650	8.163	1.00	37.34	A	O
ATOM	545	N	CYS	A	439	16.968	-2.611	6.818	1.00	37.71	A	N
ATOM	546	CA	CYS	A	439	17.418	-3.832	6.212	1.00	39.05	A	C
ATOM	547	CB	CYS	A	439	16.525	-4.996	6.669	1.00	40.75	A	C
ATOM	548	SG	CYS	A	439	16.979	-6.593	5.948	1.00	44.86	A	S
ATOM	549	C	CYS	A	439	17.194	-3.542	4.812	1.00	38.53	A	C
ATOM	550	O	CYS	A	439	16.122	-3.044	4.433	1.00	36.01	A	O
ATOM	551	N	GLU	A	440	18.234	-3.732	4.018	1.00	40.12	A	N
ATOM	552	CA	GLU	A	440	18.071	-3.412	2.568	1.00	41.76	A	C
ATOM	553	CB	GLU	A	440	19.009	-2.338	1.976	1.00	42.65	A	C
ATOM	554	CG	GLU	A	440	20.407	-2.233	2.585	1.00	49.77	A	C
ATOM	555	CD	GLU	A	440	21.551	-1.858	1.573	1.00	57.03	A	C
ATOM	556	OE1	GLU	A	440	21.230	-1.351	0.402	1.00	58.92	A	O
ATOM	557	OE2	GLU	A	440	22.784	-2.097	1.953	1.00	56.13	A	O

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Figure 2A - 10

ATOM	558	C	GLU	A	440	18.100	-4.658	1.760	1.00	40.88	A	C
ATOM	559	O	GLU	A	440	19.092	-5.403	1.692	1.00	41.05	A	O
ATOM	560	N	ALA	A	441	16.997	-4.876	1.118	1.00	39.50	A	N
ATOM	561	CA	ALA	A	441	16.958	-6.050	0.307	1.00	40.33	A	C
ATOM	562	CB	ALA	A	441	16.543	-7.203	1.172	1.00	40.44	A	C
ATOM	563	C	ALA	A	441	15.988	-5.821	-0.913	1.00	39.31	A	C
ATOM	564	O	ALA	A	441	16.116	-4.838	-1.532	1.00	36.99	A	O
ATOM	565	N	GLU	A	442	15.037	-6.707	-1.154	1.00	40.32	A	N
ATOM	566	CA	GLU	A	442	13.987	-6.511	-2.154	1.00	42.91	A	C
ATOM	567	CB	GLU	A	442	12.979	-7.682	-2.114	1.00	43.27	A	C
ATOM	568	CG	AGLU	A	442	12.130	-7.833	-0.824	0.70	42.92	A	C
ATOM	569	CG	BGLU	A	442	12.629	-8.190	-0.748	0.30	43.63	A	C
ATOM	570	CD	AGLU	A	442	12.868	-8.393	0.464	0.70	41.81	A	C
ATOM	571	CD	BGLU	A	442	11.195	-8.608	-0.681	0.30	43.62	A	C
ATOM	572	OE1	AGLU	A	442	14.130	-8.308	0.632	0.70	40.81	A	O
ATOM	573	OE1	BGLU	A	442	10.719	-8.866	0.449	0.30	45.35	A	O
ATOM	574	OE2	AGLU	A	442	12.174	-8.913	1.359	0.70	38.79	A	O
ATOM	575	OE2	BGLU	A	442	10.552	-8.636	-1.749	0.30	41.66	A	O
ATOM	576	C	GLU	A	442	13.254	-5.221	-1.933	1.00	44.04	A	C
ATOM	577	O	GLU	A	442	12.573	-4.714	-2.807	1.00	44.81	A	O
ATOM	578	N	SER	A	443	13.295	-4.725	-0.704	1.00	44.73	A	N
ATOM	579	CA	SER	A	443	12.780	-3.368	-0.441	1.00	44.85	A	C
ATOM	580	CB	SER	A	443	11.309	-3.290	-0.016	1.00	44.69	A	C
ATOM	581	OG	SER	A	443	10.552	-4.430	-0.431	1.00	45.42	A	O
ATOM	582	C	SER	A	443	13.606	-2.895	0.704	1.00	44.51	A	C
ATOM	583	O	SER	A	443	14.189	-3.679	1.449	1.00	46.61	A	O
ATOM	584	N	TRP	A	444	13.619	-1.591	0.847	1.00	43.19	A	N
ATOM	585	CA	TRP	A	444	14.286	-0.905	1.888	1.00	40.90	A	C
ATOM	586	CB	TRP	A	444	14.597	0.532	1.418	1.00	41.41	A	C
ATOM	587	CG	TRP	A	444	15.665	1.164	2.261	1.00	44.14	A	C
ATOM	588	CD1	TRP	A	444	16.981	1.145	2.044	1.00	45.71	A	C
ATOM	589	NE1	TRP	A	444	17.649	1.862	3.024	1.00	48.71	A	N
ATOM	590	CE2	TRP	A	444	16.738	2.303	3.948	1.00	48.30	A	C
ATOM	591	CD2	TRP	A	444	15.474	1.859	3.514	1.00	47.57	A	C
ATOM	592	CE3	TRP	A	444	14.339	2.196	4.296	1.00	48.48	A	C
ATOM	593	CZ3	TRP	A	444	14.525	2.983	5.490	1.00	47.21	A	C
ATOM	594	CH2	TRP	A	444	15.808	3.398	5.874	1.00	47.38	A	C
ATOM	595	CZ2	TRP	A	444	16.920	3.059	5.132	1.00	48.75	A	C
ATOM	596	C	TRP	A	444	13.346	-0.929	3.093	1.00	39.26	A	C
ATOM	597	O	TRP	A	444	12.157	-0.906	2.941	1.00	38.31	A	O
ATOM	598	N	MET	A	445	13.874	-1.006	4.302	1.00	38.06	A	N
ATOM	599	CA	MET	A	445	12.958	-1.235	5.401	1.00	36.89	A	C
ATOM	600	CB	MET	A	445	12.834	-2.749	5.613	1.00	36.43	A	C
ATOM	601	CG	MET	A	445	12.259	-3.581	4.463	1.00	37.35	A	C
ATOM	602	SD	MET	A	445	12.305	-5.478	4.759	1.00	38.75	A	S
ATOM	603	CE	MET	A	445	11.502	-5.986	3.287	1.00	39.72	A	C
ATOM	604	C	MET	A	445	13.482	-0.697	6.682	1.00	35.09	A	C
ATOM	605	O	MET	A	445	14.601	-0.970	7.060	1.00	34.94	A	O
ATOM	606	N	LEU	A	446	12.636	-0.024	7.421	1.00	33.75	A	N
ATOM	607	CA	LEU	A	446	12.995	0.372	8.779	1.00	31.44	A	C
ATOM	608	CB	LEU	A	446	12.488	1.743	9.074	1.00	28.84	A	C
ATOM	609	CG	LEU	A	446	13.206	2.656	10.054	1.00	31.25	A	C
ATOM	610	CD1	LEU	A	446	12.586	4.019	9.854	1.00	32.85	A	C
ATOM	611	CD2	LEU	A	446	13.105	2.285	11.628	1.00	32.97	A	C
ATOM	612	C	LEU	A	446	12.371	-0.634	9.686	1.00	31.17	A	C
ATOM	613	O	LEU	A	446	11.183	-0.813	9.701	1.00	31.35	A	O
ATOM	614	N	VAL	A	447	13.164	-1.260	10.521	1.00	30.77	A	N
ATOM	615	CA	VAL	A	447	12.586	-2.269	11.339	1.00	30.46	A	C
ATOM	616	CB	VAL	A	447	13.484	-3.502	11.233	1.00	31.01	A	C
ATOM	617	CG1	VAL	A	447	13.208	-4.437	12.336	1.00	27.84	A	C
ATOM	618	CG2	VAL	A	447	13.279	-4.143	9.852	1.00	29.63	A	C
ATOM	619	C	VAL	A	447	12.599	-1.772	12.754	1.00	30.86	A	C

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ATOM	620	O	VAL A 447	13.658	-1.311	13.270	1.00	29.46	A	O
ATOM	621	N	MET A 448	11.465	-1.992	13.442	1.00	30.95	A	N
ATOM	622	CA	MET A 448	11.199	-1.392	14.772	1.00	30.49	A	C
ATOM	623	CB	MET A 448	10.060	-0.391	14.563	1.00	30.18	A	C
ATOM	624	CG	MET A 448	10.441	1.027	14.262	1.00	30.25	A	C
ATOM	625	SD	MET A 448	9.045	2.000	13.615	1.00	38.04	A	S
ATOM	626	CE	MET A 448	8.264	1.140	12.435	1.00	36.04	A	C
ATOM	627	C	MET A 448	10.692	-2.376	15.853	1.00	29.81	A	C
ATOM	628	O	MET A 448	9.980	-3.340	15.510	1.00	28.77	A	O
ATOM	629	N	GLU A 449	10.929	-2.085	17.138	1.00	27.51	A	N
ATOM	630	CA	GLU A 449	10.297	-2.930	18.119	1.00	28.62	A	C
ATOM	631	CB	GLU A 449	10.667	-2.575	19.518	1.00	29.78	A	C
ATOM	632	CG	GLU A 449	10.499	-1.129	19.857	1.00	34.91	A	C
ATOM	633	CD	GLU A 449	10.639	-0.910	21.364	1.00	38.73	A	C
ATOM	634	OE1	GLU A 449	11.033	-1.927	22.052	1.00	42.29	A	O
ATOM	635	OE2	GLU A 449	10.376	0.230	21.841	1.00	33.93	A	O
ATOM	636	C	GLU A 449	8.838	-2.752	17.862	1.00	27.46	A	C
ATOM	637	O	GLU A 449	8.509	-1.746	17.347	1.00	27.49	A	O
ATOM	638	N	MET A 450	8.001	-3.786	18.028	1.00	26.05	A	N
ATOM	639	CA	MET A 450	6.580	-3.720	17.757	1.00	27.92	A	C
ATOM	640	CB	MET A 450	6.062	-5.120	17.496	1.00	30.51	A	C
ATOM	641	CG	MET A 450	4.493	-5.274	17.600	1.00	31.44	A	C
ATOM	642	SD	MET A 450	4.006	-5.067	15.917	1.00	33.93	A	S
ATOM	643	CE	MET A 450	2.053	-4.803	16.012	1.00	29.52	A	C
ATOM	644	C	MET A 450	5.713	-3.262	18.894	1.00	28.82	A	C
ATOM	645	O	MET A 450	5.846	-3.751	20.078	1.00	30.27	A	O
ATOM	646	N	ALA A 451	4.833	-2.348	18.621	1.00	27.56	A	N
ATOM	647	CA	ALA A 451	3.908	-2.088	19.704	1.00	30.36	A	C
ATOM	648	CB	ALA A 451	3.868	-0.552	20.198	1.00	30.97	A	C
ATOM	649	C	ALA A 451	2.515	-2.659	19.397	1.00	29.49	A	C
ATOM	650	O	ALA A 451	1.767	-2.097	18.634	1.00	26.89	A	O
ATOM	651	N	GLU A 452	2.230	-3.743	20.100	1.00	30.57	A	N
ATOM	652	CA	GLU A 452	1.155	-4.664	19.826	1.00	32.87	A	C
ATOM	653	CB	GLU A 452	1.262	-5.913	20.745	1.00	34.07	A	C
ATOM	654	CG	GLU A 452	2.582	-6.697	20.830	1.00	37.88	A	C
ATOM	655	CD	GLU A 452	2.860	-7.667	19.543	1.00	42.72	A	C
ATOM	656	OE1	GLU A 452	1.998	-7.763	18.562	1.00	39.51	A	O
ATOM	657	OE2	GLU A 452	3.950	-8.368	19.539	1.00	39.62	A	O
ATOM	658	C	GLU A 452	-0.224	-4.128	19.952	1.00	33.40	A	C
ATOM	659	O	GLU A 452	-1.073	-4.694	19.362	1.00	35.93	A	O
ATOM	660	N	LEU A 453	-0.520	-3.099	20.736	1.00	32.98	A	N
ATOM	661	CA	LEU A 453	-1.900	-2.698	20.791	1.00	31.73	A	C
ATOM	662	CB	LEU A 453	-2.341	-2.356	22.184	1.00	31.16	A	C
ATOM	663	CG	LEU A 453	-2.179	-3.551	23.130	1.00	32.01	A	C
ATOM	664	CD1	LEU A 453	-2.846	-3.283	24.456	1.00	29.55	A	C
ATOM	665	CD2	LEU A 453	-2.701	-4.859	22.459	1.00	32.76	A	C
ATOM	666	C	LEU A 453	-2.240	-1.588	19.909	1.00	32.02	A	C
ATOM	667	O	LEU A 453	-3.407	-1.100	19.957	1.00	30.59	A	O
ATOM	668	N	GLY A 454	-1.249	-1.147	19.124	1.00	31.47	A	N
ATOM	669	CA	GLY A 454	-1.499	-0.079	18.151	1.00	31.92	A	C
ATOM	670	C	GLY A 454	-1.508	1.358	18.713	1.00	32.17	A	C
ATOM	671	O	GLY A 454	-1.116	1.595	19.932	1.00	32.68	A	O
ATOM	672	N	PRO A 455	-2.030	2.273	17.879	1.00	29.76	A	N
ATOM	673	CA	PRO A 455	-2.106	3.702	18.203	1.00	30.46	A	C
ATOM	674	CB	PRO A 455	-2.618	4.340	16.879	1.00	29.47	A	C
ATOM	675	CG	PRO A 455	-2.485	3.241	15.874	1.00	28.34	A	C
ATOM	676	CD	PRO A 455	-2.649	1.975	16.585	1.00	28.37	A	C
ATOM	677	C	PRO A 455	-3.095	4.089	19.330	1.00	30.10	A	C
ATOM	678	O	PRO A 455	-4.190	3.578	19.393	1.00	27.95	A	O
ATOM	679	N	LEU A 456	-2.686	5.051	20.151	1.00	30.20	A	N
ATOM	680	CA	LEU A 456	-3.505	5.543	21.263	1.00	29.99	A	C
ATOM	681	CB	LEU A 456	-2.783	6.666	22.030	1.00	30.03	A	C

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Figure 2A - 12

ATOM	682	CG	LEU	A	456	-3.510	7.068	23.266	1.00	29.09	A	C
ATOM	683	CD1	LEU	A	456	-3.673	5.962	24.423	1.00	24.77	A	C
ATOM	684	CD2	LEU	A	456	-2.796	8.259	23.717	1.00	28.62	A	C
ATOM	685	C	LEU	A	456	-4.946	5.936	20.895	1.00	28.31	A	C
ATOM	686	O	LEU	A	456	-5.885	5.423	21.480	1.00	27.33	A	O
ATOM	687	N	ASN	A	457	-5.127	6.796	19.919	1.00	25.93	A	N
ATOM	688	CA	ASN	A	457	-6.460	7.099	19.509	1.00	26.38	A	C
ATOM	689	CB	ASN	A	457	-6.489	8.240	18.543	1.00	26.53	A	C
ATOM	690	CG	ASN	A	457	-5.867	7.947	17.211	1.00	28.24	A	C
ATOM	691	OD1	ASN	A	457	-5.288	6.893	16.948	1.00	30.24	A	O
ATOM	692	ND2	ASN	A	457	-5.973	8.899	16.350	1.00	27.30	A	N
ATOM	693	C	ASN	A	457	-7.366	5.914	19.112	1.00	27.00	A	C
ATOM	694	O	ASN	A	457	-8.479	5.782	19.661	1.00	25.48	A	O
ATOM	695	N	LYS	A	458	-6.922	5.042	18.211	1.00	26.77	A	N
ATOM	696	CA	LYS	A	458	-7.798	3.949	17.865	1.00	29.75	A	C
ATOM	697	CB	LYS	A	458	-7.207	3.083	16.808	1.00	30.42	A	C
ATOM	698	CG	LYS	A	458	-7.389	3.574	15.424	1.00	38.29	A	C
ATOM	699	CD	LYS	A	458	-6.074	3.461	14.566	1.00	45.31	A	C
ATOM	700	CE	LYS	A	458	-6.340	3.336	13.031	1.00	48.40	A	C
ATOM	701	NZ	LYS	A	458	-5.408	4.199	12.162	1.00	45.31	A	N
ATOM	702	C	LYS	A	458	-8.110	3.121	19.076	1.00	29.23	A	C
ATOM	703	O	LYS	A	458	-9.226	2.640	19.252	1.00	30.31	A	O
ATOM	704	N	TYR	A	459	-7.123	2.910	19.915	1.00	27.87	A	N
ATOM	705	CA	TYR	A	459	-7.299	2.031	21.059	1.00	27.89	A	C
ATOM	706	CB	TYR	A	459	-5.985	1.778	21.808	1.00	26.46	A	C
ATOM	707	CG	TYR	A	459	-6.176	1.037	23.105	1.00	26.74	A	C
ATOM	708	CD1	TYR	A	459	-6.058	-0.311	23.120	1.00	28.26	A	C
ATOM	709	CE1	TYR	A	459	-6.341	-1.007	24.146	1.00	32.30	A	C
ATOM	710	CZ	TYR	A	459	-6.567	-0.393	25.305	1.00	35.60	A	C
ATOM	711	OH	TYR	A	459	-6.636	-1.244	26.341	1.00	40.84	A	O
ATOM	712	CE2	TYR	A	459	-6.634	0.990	25.420	1.00	32.85	A	C
ATOM	713	CD2	TYR	A	459	-6.443	1.686	24.302	1.00	28.08	A	C
ATOM	714	C	TYR	A	459	-8.392	2.559	22.025	1.00	28.48	A	C
ATOM	715	O	TYR	A	459	-9.208	1.795	22.579	1.00	28.47	A	O
ATOM	716	N	LEU	A	460	-8.400	3.863	22.219	1.00	28.12	A	N
ATOM	717	CA	LEU	A	460	-9.279	4.428	23.156	1.00	28.68	A	C
ATOM	718	CB	LEU	A	460	-8.781	5.746	23.686	1.00	27.83	A	C
ATOM	719	CG	LEU	A	460	-7.554	5.845	24.537	1.00	27.77	A	C
ATOM	720	CD1	LEU	A	460	-7.223	7.307	24.752	1.00	24.85	A	C
ATOM	721	CD2	LEU	A	460	-7.690	5.158	25.887	1.00	29.17	A	C
ATOM	722	C	LEU	A	460	-10.597	4.557	22.454	1.00	29.67	A	C
ATOM	723	O	LEU	A	460	-11.647	4.390	23.123	1.00	28.14	A	O
ATOM	724	N	GLN	A	461	-10.596	4.799	21.124	1.00	30.58	A	N
ATOM	725	CA	GLN	A	461	-11.892	4.800	20.423	1.00	31.45	A	C
ATOM	726	CB	GLN	A	461	-11.798	5.164	18.922	1.00	31.63	A	C
ATOM	727	CG	AGLN	A	461	-11.689	6.678	18.659	0.20	32.26	A	C
ATOM	728	CG	BGLN	A	461	-11.133	6.613	18.505	0.80	33.76	A	C
ATOM	729	CD	AGLN	A	461	-13.047	7.386	18.567	0.20	33.75	A	C
ATOM	730	CD	BGLN	A	461	-10.684	6.709	16.929	0.80	38.32	A	C
ATOM	731	OE1AGLN	A	461	-13.914	7.016	17.761	0.20	32.93	A	O	
ATOM	732	OE1BGLN	A	461	-10.934	5.773	16.121	0.80	41.14	A	O	
ATOM	733	NE2AGLN	A	461	-13.224	8.415	19.387	0.20	34.82	A	N	
ATOM	734	NE2BGLN	A	461	-10.064	7.835	16.532	0.80	38.06	A	N	
ATOM	735	C	GLN	A	461	-12.581	3.455	20.618	1.00	31.48	A	C
ATOM	736	O	GLN	A	461	-13.786	3.385	20.728	1.00	32.12	A	O
ATOM	737	N	GLN	A	462	-11.834	2.360	20.637	1.00	31.61	A	N
ATOM	738	CA	GLN	A	462	-12.448	1.039	20.784	1.00	31.50	A	C
ATOM	739	CB	GLN	A	462	-11.632	0.039	19.985	1.00	32.94	A	C
ATOM	740	CG	AGLN	A	462	-12.379	-0.661	18.855	0.50	35.36	A	C
ATOM	741	CG	BGLN	A	462	-11.578	0.562	18.527	0.50	34.33	A	C
ATOM	742	CD	AGLN	A	462	-11.999	-0.073	17.536	0.50	37.73	A	C
ATOM	743	CD	BGLN	A	462	-12.984	0.700	17.902	0.50	35.59	A	C

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Figure 2A - 13

ATOM	744	OE1AGLN	A	462	-10.855	0.359	17.370	0.50	37.57	A	O	
ATOM	745	OE1BGLN	A	462	-13.423	1.798	17.428	0.50	32.32	A	O	
ATOM	746	NE2AGLN	A	462	-12.952	-0.003	16.602	0.50	39.96	A	N	
ATOM	747	NE2BGLN	A	462	-13.682	-0.438	17.861	0.50	36.84	A	N	
ATOM	748	C	GLN	A	462	-12.537	0.511	22.195	1.00	29.83	A	C
ATOM	749	O	GLN	A	462	-12.936	-0.682	22.404	1.00	26.71	A	O
ATOM	750	N	ASN	A	463	-12.119	1.334	23.164	1.00	28.43	A	N
ATOM	751	CA	ASN	A	463	-12.115	0.846	24.579	1.00	28.96	A	C
ATOM	752	CB	ASN	A	463	-10.747	0.307	24.962	1.00	27.90	A	C
ATOM	753	CG	ASN	A	463	-10.430	-1.025	24.330	1.00	31.24	A	C
ATOM	754	OD1	ASN	A	463	-10.896	-2.020	24.826	1.00	34.65	A	O
ATOM	755	ND2	ASN	A	463	-9.575	-1.070	23.258	1.00	29.89	A	N
ATOM	756	C	ASN	A	463	-12.494	2.002	25.447	1.00	29.08	A	C
ATOM	757	O	ASN	A	463	-11.650	2.637	26.052	1.00	27.75	A	O
ATOM	758	N	ARG	A	464	-13.770	2.293	25.486	1.00	30.22	A	N
ATOM	759	CA	ARG	A	464	-14.302	3.474	26.103	1.00	33.81	A	C
ATOM	760	CB	ARG	A	464	-15.601	3.867	25.400	1.00	35.64	A	C
ATOM	761	CG	ARG	A	464	-15.259	4.641	24.104	1.00	41.33	A	C
ATOM	762	CD	ARG	A	464	-16.411	4.919	23.095	1.00	50.05	A	C
ATOM	763	NE	ARG	A	464	-15.820	5.361	21.822	1.00	55.81	A	N
ATOM	764	CZ	ARG	A	464	-16.505	5.827	20.769	1.00	60.17	A	C
ATOM	765	NH1	ARG	A	464	-17.832	5.947	20.809	1.00	62.01	A	N
ATOM	766	NH2	ARG	A	464	-15.859	6.197	19.669	1.00	61.43	A	N
ATOM	767	C	ARG	A	464	-14.497	3.425	27.597	1.00	34.41	A	C
ATOM	768	O	ARG	A	464	-15.037	4.378	28.182	1.00	34.05	A	O
ATOM	769	N	HIS	A	465	-14.009	2.375	28.209	1.00	34.39	A	N
ATOM	770	CA	HIS	A	465	-14.170	2.280	29.625	1.00	37.55	A	C
ATOM	771	CB	HIS	A	465	-15.121	1.123	29.973	1.00	39.65	A	C
ATOM	772	CG	HIS	A	465	-16.467	1.320	29.332	1.00	48.44	A	C
ATOM	773	ND1	HIS	A	465	-16.942	0.512	28.313	1.00	53.58	A	N
ATOM	774	CE1	HIS	A	465	-18.090	1.017	27.860	1.00	55.95	A	C
ATOM	775	NE2	HIS	A	465	-18.355	2.142	28.517	1.00	53.41	A	N
ATOM	776	CD2	HIS	A	465	-17.359	2.355	29.440	1.00	53.01	A	C
ATOM	777	C	HIS	A	465	-12.843	2.245	30.318	1.00	36.35	A	C
ATOM	778	O	HIS	A	465	-12.785	1.921	31.510	1.00	35.68	A	O
ATOM	779	N	VAL	A	466	-11.783	2.566	29.561	1.00	33.28	A	N
ATOM	780	CA	VAL	A	466	-10.492	2.677	30.149	1.00	30.86	A	C
ATOM	781	CB	VAL	A	466	-9.452	3.051	29.099	1.00	29.85	A	C
ATOM	782	CG1	VAL	A	466	-8.184	3.555	29.745	1.00	26.29	A	C
ATOM	783	CG2	VAL	A	466	-9.056	1.789	28.342	1.00	30.63	A	C
ATOM	784	C	VAL	A	466	-10.593	3.725	31.247	1.00	31.45	A	C
ATOM	785	O	VAL	A	466	-11.256	4.739	31.047	1.00	29.64	A	O
ATOM	786	N	LYS	A	467	-9.882	3.538	32.377	1.00	31.85	A	N
ATOM	787	CA	LYS	A	467	-10.139	4.408	33.487	1.00	33.27	A	C
ATOM	788	CB	LYS	A	467	-9.932	3.643	34.798	1.00	34.58	A	C
ATOM	789	CG	LYS	A	467	-10.694	2.281	34.875	1.00	37.15	A	C
ATOM	790	CD	LYS	A	467	-11.888	2.333	35.796	1.00	43.80	A	C
ATOM	791	CE	LYS	A	467	-12.461	0.840	36.003	1.00	51.10	A	C
ATOM	792	NZ	LYS	A	467	-11.336	-0.239	36.352	1.00	53.24	A	N
ATOM	793	C	LYS	A	467	-9.215	5.601	33.421	1.00	32.82	A	C
ATOM	794	O	LYS	A	467	-8.156	5.503	32.813	1.00	32.18	A	O
ATOM	795	N	ASP	A	468	-9.609	6.672	34.113	1.00	31.43	A	N
ATOM	796	CA	ASP	A	468	-8.946	7.947	34.123	1.00	32.95	A	C
ATOM	797	CB	ASP	A	468	-9.696	8.936	35.062	1.00	33.46	A	C
ATOM	798	CG	ASP	A	468	-10.837	9.674	34.384	1.00	36.56	A	C
ATOM	799	OD1	ASP	A	468	-10.740	9.889	33.129	1.00	37.92	A	O
ATOM	800	OD2	ASP	A	468	-11.897	10.074	35.031	1.00	37.14	A	O
ATOM	801	C	ASP	A	468	-7.524	7.716	34.634	1.00	31.27	A	C
ATOM	802	O	ASP	A	468	-6.435	8.256	34.161	1.00	27.94	A	O
ATOM	803	N	LYS	A	469	-7.558	6.893	35.639	1.00	31.16	A	N
ATOM	804	CA	LYS	A	469	-6.295	6.545	36.187	1.00	32.39	A	C
ATOM	805	CB	LYS	A	469	-6.392	5.539	37.335	1.00	32.33	A	C

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ATOM	806	CG	LYS	A	469	-5.032	5.277	37.874	1.00	35.44	A	C
ATOM	807	CD	LYS	A	469	-5.047	4.887	39.382	1.00	41.14	A	C
ATOM	808	CE	LYS	A	469	-4.328	3.532	39.753	1.00	42.47	A	C
ATOM	809	NZ	LYS	A	469	-5.284	2.316	40.028	1.00	42.30	A	N
ATOM	810	C	LYS	A	469	-5.454	6.005	35.019	1.00	29.32	A	C
ATOM	811	O	LYS	A	469	-4.382	6.489	34.819	1.00	29.53	A	O
ATOM	812	N	ASN	A	470	-5.938	5.022	34.278	1.00	25.80	A	N
ATOM	813	CA	ASN	A	470	-5.109	4.432	33.253	1.00	25.30	A	C
ATOM	814	CB	ASN	A	470	-5.840	3.309	32.632	1.00	23.14	A	C
ATOM	815	CG	ASN	A	470	-5.010	2.377	31.804	1.00	22.63	A	C
ATOM	816	OD1	ASN	A	470	-5.497	1.328	31.602	1.00	26.10	A	O
ATOM	817	ND2	ASN	A	470	-3.743	2.627	31.509	1.00	16.19	A	N
ATOM	818	C	ASN	A	470	-4.773	5.516	32.144	1.00	26.10	A	C
ATOM	819	O	ASN	A	470	-3.703	5.495	31.538	1.00	26.25	A	O
ATOM	820	N	ILE	A	471	-5.673	6.429	31.864	1.00	24.97	A	N
ATOM	821	CA	ILE	A	471	-5.257	7.418	30.993	1.00	26.84	A	C
ATOM	822	CB	ILE	A	471	-6.434	8.126	30.510	1.00	27.88	A	C
ATOM	823	CG1	ILE	A	471	-7.303	7.087	29.836	1.00	25.97	A	C
ATOM	824	CD1	ILE	A	471	-8.493	7.680	29.481	1.00	28.95	A	C
ATOM	825	CG2	ILE	A	471	-5.973	9.275	29.594	1.00	22.75	A	C
ATOM	826	C	ILE	A	471	-4.180	8.386	31.521	1.00	28.18	A	C
ATOM	827	O	ILE	A	471	-3.337	8.826	30.773	1.00	27.68	A	O
ATOM	828	N	ILE	A	472	-4.158	8.685	32.828	1.00	28.56	A	N
ATOM	829	CA	ILE	A	472	-3.133	9.558	33.318	1.00	26.96	A	C
ATOM	830	CB	ILE	A	472	-3.435	9.926	34.784	1.00	27.63	A	C
ATOM	831	CG1	ILE	A	472	-4.666	10.858	34.834	1.00	28.56	A	C
ATOM	832	CD1	ILE	A	472	-5.344	10.926	36.247	1.00	28.39	A	C
ATOM	833	CG2	ILE	A	472	-2.308	10.605	35.446	1.00	23.72	A	C
ATOM	834	C	ILE	A	472	-1.838	8.855	33.182	1.00	26.80	A	C
ATOM	835	O	ILE	A	472	-0.816	9.422	32.804	1.00	27.42	A	O
ATOM	836	N	GLU	A	473	-1.856	7.584	33.463	1.00	26.02	A	N
ATOM	837	CA	GLU	A	473	-0.610	6.846	33.437	1.00	25.63	A	C
ATOM	838	CB	GLU	A	473	-0.860	5.372	33.870	1.00	26.20	A	C
ATOM	839	CG	GLU	A	473	0.335	4.410	33.793	1.00	28.75	A	C
ATOM	840	CD	GLU	A	473	-0.085	2.901	33.849	1.00	34.58	A	C
ATOM	841	OE1	GLU	A	473	-1.173	2.505	33.289	1.00	31.33	A	O
ATOM	842	OE2	GLU	A	473	0.700	2.069	34.449	1.00	37.48	A	O
ATOM	843	C	GLU	A	473	0.046	6.891	32.061	1.00	23.54	A	C
ATOM	844	O	GLU	A	473	1.190	7.029	31.953	1.00	22.74	A	O
ATOM	845	N	LEU	A	474	-0.706	6.695	31.014	1.00	22.95	A	N
ATOM	846	CA	LEU	A	474	-0.215	6.645	29.679	1.00	21.98	A	C
ATOM	847	CB	LEU	A	474	-1.362	6.213	28.634	1.00	21.67	A	C
ATOM	848	CG	LEU	A	474	-1.882	4.795	28.778	1.00	21.33	A	C
ATOM	849	CD1	LEU	A	474	-3.238	4.576	28.186	1.00	19.07	A	C
ATOM	850	CD2	LEU	A	474	-0.826	3.757	28.342	1.00	20.55	A	C
ATOM	851	C	LEU	A	474	0.240	7.976	29.303	1.00	21.73	A	C
ATOM	852	O	LEU	A	474	1.214	8.007	28.671	1.00	19.80	A	O
ATOM	853	N	VAL	A	475	-0.494	9.079	29.629	1.00	22.40	A	N
ATOM	854	CA	VAL	A	475	-0.028	10.405	29.177	1.00	22.09	A	C
ATOM	855	CB	VAL	A	475	-1.103	11.601	28.993	1.00	21.76	A	C
ATOM	856	CG1	VAL	A	475	-2.200	11.241	28.089	1.00	22.57	A	C
ATOM	857	CG2	VAL	A	475	-1.702	12.032	30.251	1.00	21.59	A	C
ATOM	858	C	VAL	A	475	1.184	10.842	29.966	1.00	23.17	A	C
ATOM	859	O	VAL	A	475	2.043	11.560	29.374	1.00	24.75	A	O
ATOM	860	N	HIS	A	476	1.251	10.518	31.271	1.00	21.80	A	N
ATOM	861	CA	HIS	A	476	2.500	10.729	32.015	1.00	23.38	A	C
ATOM	862	CB	HIS	A	476	2.407	10.219	33.483	1.00	22.70	A	C
ATOM	863	CG	HIS	A	476	3.666	10.438	34.223	1.00	24.35	A	C
ATOM	864	ND1	HIS	A	476	4.426	9.401	34.736	1.00	24.81	A	N
ATOM	865	CE1	HIS	A	476	5.527	9.879	35.249	1.00	24.49	A	C
ATOM	866	NE2	HIS	A	476	5.544	11.181	35.044	1.00	26.37	A	N
ATOM	867	CD2	HIS	A	476	4.402	11.557	34.381	1.00	24.33	A	C

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## Figure 2A - 15

ATOM	868	C	HIS	A	476	3.687	10.024	31.350	1.00	23.20	A	C
ATOM	869	O	HIS	A	476	4.767	10.540	31.226	1.00	21.18	A	O
ATOM	870	N	GLN	A	477	3.446	8.785	30.972	1.00	24.64	A	N
ATOM	871	CA	GLN	A	477	4.437	8.118	30.105	1.00	27.01	A	C
ATOM	872	CB	GLN	A	477	4.045	6.698	29.671	1.00	26.30	A	C
ATOM	873	CG	GLN	A	477	3.877	5.787	30.884	1.00	27.41	A	C
ATOM	874	CD	GLN	A	477	3.504	4.355	30.569	1.00	28.90	A	C
ATOM	875	OE1	GLN	A	477	3.058	4.058	29.453	1.00	23.96	A	O
ATOM	876	NE2	GLN	A	477	3.766	3.420	31.564	1.00	30.38	A	N
ATOM	877	C	GLN	A	477	4.891	8.933	28.889	1.00	27.32	A	C
ATOM	878	O	GLN	A	477	6.103	9.043	28.638	1.00	28.19	A	O
ATOM	879	N	VAL	A	478	3.975	9.555	28.172	1.00	26.15	A	N
ATOM	880	CA	VAL	A	478	4.419	10.246	26.959	1.00	24.16	A	C
ATOM	881	CB	VAL	A	478	3.204	10.605	26.095	1.00	25.14	A	C
ATOM	882	CG1	VAL	A	478	3.584	11.649	24.954	1.00	23.94	A	C
ATOM	883	CG2	VAL	A	478	2.520	9.308	25.478	1.00	18.46	A	C
ATOM	884	C	VAL	A	478	5.194	11.453	27.427	1.00	24.65	A	C
ATOM	885	O	VAL	A	478	6.130	11.909	26.773	1.00	22.86	A	O
ATOM	886	N	SER	A	479	4.864	11.927	28.639	1.00	23.23	A	N
ATOM	887	CA	SER	A	479	5.542	13.089	29.066	1.00	24.08	A	C
ATOM	888	CB	SER	A	479	4.809	13.795	30.174	1.00	23.46	A	C
ATOM	889	OG	SER	A	479	4.970	13.136	31.450	1.00	23.37	A	O
ATOM	890	C	SER	A	479	7.020	12.743	29.472	1.00	26.82	A	C
ATOM	891	O	SER	A	479	7.959	13.611	29.293	1.00	27.31	A	O
ATOM	892	N	MET	A	480	7.259	11.529	29.950	1.00	25.22	A	N
ATOM	893	CA	MET	A	480	8.609	11.220	30.311	1.00	27.73	A	C
ATOM	894	CB	MET	A	480	8.613	9.937	31.153	1.00	29.14	A	C
ATOM	895	CG	MET	A	480	8.239	10.184	32.602	1.00	31.02	A	C
ATOM	896	SD	MET	A	480	8.415	8.676	33.604	1.00	32.50	A	S
ATOM	897	CE	MET	A	480	6.962	7.731	33.091	1.00	32.71	A	C
ATOM	898	C	MET	A	480	9.415	10.999	29.056	1.00	27.61	A	C
ATOM	899	O	MET	A	480	10.593	11.325	28.978	1.00	27.43	A	O
ATOM	900	N	GLY	A	481	8.756	10.524	28.021	1.00	26.61	A	N
ATOM	901	CA	GLY	A	481	9.435	10.332	26.757	1.00	24.74	A	C
ATOM	902	C	GLY	A	481	9.742	11.707	26.208	1.00	24.37	A	C
ATOM	903	O	GLY	A	481	10.837	11.949	25.674	1.00	23.10	A	O
ATOM	904	N	MET	A	482	8.796	12.624	26.322	1.00	22.93	A	N
ATOM	905	CA	MET	A	482	9.019	13.881	25.664	1.00	22.10	A	C
ATOM	906	CB	MET	A	482	7.747	14.627	25.516	1.00	20.75	A	C
ATOM	907	CG	MET	A	482	6.834	14.093	24.500	1.00	21.81	A	C
ATOM	908	SD	MET	A	482	7.628	14.003	22.833	1.00	25.96	A	S
ATOM	909	CE	MET	A	482	8.064	15.712	22.563	1.00	26.88	A	C
ATOM	910	C	MET	A	482	10.058	14.676	26.475	1.00	22.96	A	C
ATOM	911	O	MET	A	482	10.773	15.516	25.957	1.00	20.44	A	O
ATOM	912	N	LYS	A	483	10.147	14.399	27.773	1.00	22.97	A	N
ATOM	913	CA	LYS	A	483	11.124	15.102	28.541	1.00	24.41	A	C
ATOM	914	CB	LYS	A	483	10.783	15.064	30.019	1.00	24.82	A	C
ATOM	915	CG	LYS	A	483	11.986	15.033	30.972	1.00	24.42	A	C
ATOM	916	CD	LYS	A	483	11.545	15.043	32.474	1.00	27.12	A	C
ATOM	917	CE	LYS	A	483	12.848	15.173	33.374	1.00	32.83	A	C
ATOM	918	NZ	LYS	A	483	12.340	15.334	34.698	1.00	35.64	A	N
ATOM	919	C	LYS	A	483	12.588	14.594	28.210	1.00	24.86	A	C
ATOM	920	O	LYS	A	483	13.522	15.369	28.154	1.00	23.57	A	O
ATOM	921	N	TYR	A	484	12.753	13.303	27.986	1.00	25.26	A	N
ATOM	922	CA	TYR	A	484	13.982	12.866	27.401	1.00	28.14	A	C
ATOM	923	CB	TYR	A	484	13.976	11.332	27.384	1.00	29.62	A	C
ATOM	924	CG	TYR	A	484	14.979	10.723	26.409	1.00	28.85	A	C
ATOM	925	CD1	TYR	A	484	14.643	10.548	25.045	1.00	26.89	A	C
ATOM	926	CE1	TYR	A	484	15.603	10.016	24.143	1.00	28.98	A	C
ATOM	927	CZ	TYR	A	484	16.936	9.685	24.643	1.00	27.82	A	C
ATOM	928	OH	TYR	A	484	17.827	9.151	23.766	1.00	26.55	A	O
ATOM	929	CE2	TYR	A	484	17.265	9.844	25.942	1.00	23.89	A	C

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## Figure 2A - 16

ATOM	930	CD2	TYR	A	484	16.288	10.400	26.833	1.00	27.18	A	C
ATOM	931	C	TYR	A	484	14.270	13.469	25.962	1.00	29.20	A	C
ATOM	932	O	TYR	A	484	15.335	13.941	25.648	1.00	29.76	A	O
ATOM	933	N	LEU	A	485	13.314	13.489	25.098	1.00	30.97	A	N
ATOM	934	CA	LEU	A	485	13.536	14.145	23.820	1.00	33.15	A	C
ATOM	935	CB	LEU	A	485	12.260	14.160	23.078	1.00	32.58	A	C
ATOM	936	CG	LEU	A	485	12.645	13.646	21.757	1.00	35.52	A	C
ATOM	937	CD1	LEU	A	485	13.154	12.176	21.787	1.00	34.25	A	C
ATOM	938	CD2	LEU	A	485	11.366	13.743	21.050	1.00	36.64	A	C
ATOM	939	C	LEU	A	485	13.951	15.580	23.964	1.00	34.05	A	C
ATOM	940	O	LEU	A	485	14.789	16.027	23.243	1.00	33.88	A	O
ATOM	941	N	GLU	A	486	13.369	16.289	24.915	1.00	35.45	A	N
ATOM	942	CA	GLU	A	486	13.699	17.693	25.112	1.00	38.20	A	C
ATOM	943	CB	GLU	A	486	12.857	18.339	26.251	1.00	38.10	A	C
ATOM	944	CG	GLU	A	486	13.112	19.817	26.538	1.00	40.40	A	C
ATOM	945	CD	GLU	A	486	12.094	20.440	27.524	1.00	47.04	A	C
ATOM	946	OE1	GLU	A	486	12.363	20.556	28.736	1.00	45.29	A	O
ATOM	947	OE2	GLU	A	486	10.973	20.850	27.088	1.00	50.30	A	O
ATOM	948	C	GLU	A	486	15.162	17.728	25.575	1.00	38.09	A	C
ATOM	949	O	GLU	A	486	15.973	18.550	25.135	1.00	36.90	A	O
ATOM	950	N	GLU	A	487	15.467	16.782	26.448	1.00	37.80	A	N
ATOM	951	CA	GLU	A	487	16.757	16.745	27.070	1.00	38.61	A	C
ATOM	952	CB	GLU	A	487	16.689	15.687	28.103	1.00	40.98	A	C
ATOM	953	CG	GLU	A	487	17.189	16.020	29.481	1.00	46.47	A	C
ATOM	954	CD	GLU	A	487	16.758	14.896	30.418	1.00	53.18	A	C
ATOM	955	OE1	GLU	A	487	15.703	15.011	31.114	1.00	51.80	A	O
ATOM	956	OE2	GLU	A	487	17.458	13.842	30.366	1.00	58.53	A	O
ATOM	957	C	GLU	A	487	17.823	16.424	26.006	1.00	36.97	A	C
ATOM	958	O	GLU	A	487	18.885	16.943	26.087	1.00	36.22	A	O
ATOM	959	N	SER	A	488	17.496	15.666	24.965	1.00	34.68	A	N
ATOM	960	CA	SER	A	488	18.434	15.381	23.933	1.00	33.48	A	C
ATOM	961	CB	SER	A	488	18.139	13.977	23.387	1.00	34.09	A	C
ATOM	962	OG	SER	A	488	17.627	13.126	24.399	1.00	33.83	A	O
ATOM	963	C	SER	A	488	18.370	16.416	22.817	1.00	33.55	A	C
ATOM	964	O	SER	A	488	18.836	16.262	21.682	1.00	33.07	A	O
ATOM	965	N	ASN	A	489	17.711	17.488	23.103	1.00	33.52	A	N
ATOM	966	CA	ASN	A	489	17.653	18.512	22.106	1.00	32.76	A	C
ATOM	967	CB	ASN	A	489	18.932	19.349	22.126	1.00	33.39	A	C
ATOM	968	CG	ASN	A	489	18.926	20.222	23.329	1.00	34.22	A	C
ATOM	969	OD1	ASN	A	489	18.085	21.101	23.447	1.00	35.35	A	O
ATOM	970	ND2	ASN	A	489	19.730	19.901	24.308	1.00	33.50	A	N
ATOM	971	C	ASN	A	489	17.105	18.085	20.749	1.00	31.40	A	C
ATOM	972	O	ASN	A	489	17.550	18.556	19.650	1.00	29.21	A	O
ATOM	973	N	PHE	A	490	16.054	17.265	20.887	1.00	29.59	A	N
ATOM	974	CA	PHE	A	490	15.241	16.934	19.754	1.00	30.63	A	C
ATOM	975	CB	PHE	A	490	15.142	15.426	19.608	1.00	30.30	A	C
ATOM	976	CG	PHE	A	490	16.262	14.790	18.822	1.00	29.98	A	C
ATOM	977	CD1	PHE	A	490	16.210	14.697	17.480	1.00	30.13	A	C
ATOM	978	CE1	PHE	A	490	17.224	14.049	16.789	1.00	33.15	A	C
ATOM	979	CZ	PHE	A	490	18.269	13.487	17.454	1.00	32.63	A	C
ATOM	980	CE2	PHE	A	490	18.331	13.567	18.791	1.00	32.39	A	C
ATOM	981	CD2	PHE	A	490	17.321	14.215	19.479	1.00	33.25	A	C
ATOM	982	C	PHE	A	490	13.793	17.580	19.784	1.00	30.34	A	C
ATOM	983	O	PHE	A	490	13.201	17.701	20.853	1.00	28.87	A	O
ATOM	984	N	VAL	A	491	13.250	17.976	18.619	1.00	28.75	A	N
ATOM	985	CA	VAL	A	491	11.841	18.338	18.542	1.00	28.81	A	C
ATOM	986	CB	VAL	A	491	11.558	19.713	17.969	1.00	28.91	A	C
ATOM	987	CG1	VAL	A	491	12.204	20.678	18.813	1.00	30.01	A	C
ATOM	988	CG2	VAL	A	491	12.067	19.774	16.373	1.00	25.43	A	C
ATOM	989	C	VAL	A	491	11.106	17.325	17.661	1.00	29.07	A	C
ATOM	990	O	VAL	A	491	11.542	17.004	16.521	1.00	28.37	A	O
ATOM	991	N	HIS	A	492	9.939	16.944	18.148	1.00	28.04	A	N



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ATOM	992	CA	HIS	A	492	9.195	15.921	17.499	1.00	27.82	A	C
ATOM	993	CB	HIS	A	492	8.271	15.184	18.453	1.00	27.10	A	C
ATOM	994	CG	HIS	A	492	7.580	14.019	17.828	1.00	26.29	A	C
ATOM	995	ND1	HIS	A	492	6.500	14.166	16.966	1.00	25.41	A	N
ATOM	996	CE1	HIS	A	492	6.090	12.964	16.607	1.00	25.87	A	C
ATOM	997	NE2	HIS	A	492	6.893	12.053	17.157	1.00	23.04	A	N
ATOM	998	CD2	HIS	A	492	7.795	12.685	17.965	1.00	21.77	A	C
ATOM	999	C	HIS	A	492	8.446	16.415	16.290	1.00	28.39	A	C
ATOM	1000	O	HIS	A	492	8.564	15.819	15.249	1.00	27.23	A	O
ATOM	1001	N	ARG	A	493	7.627	17.450	16.478	1.00	28.09	A	N
ATOM	1002	CA	ARG	A	493	6.920	18.005	15.402	1.00	27.70	A	C
ATOM	1003	CB	ARG	A	493	7.938	18.398	14.292	1.00	29.03	A	C
ATOM	1004	CG	ARG	A	493	8.703	19.697	14.653	1.00	29.90	A	C
ATOM	1005	CD	ARG	A	493	9.671	20.133	13.555	1.00	34.10	A	C
ATOM	1006	NE	ARG	A	493	8.945	20.755	12.463	1.00	37.86	A	N
ATOM	1007	CZ	ARG	A	493	8.985	20.385	11.199	1.00	35.58	A	C
ATOM	1008	NH1	ARG	A	493	9.749	19.347	10.850	1.00	31.85	A	N
ATOM	1009	NH2	ARG	A	493	8.233	21.049	10.325	1.00	33.13	A	N
ATOM	1010	C	ARG	A	493	5.735	17.219	14.821	1.00	27.08	A	C
ATOM	1011	O	ARG	A	493	5.161	17.593	13.805	1.00	26.21	A	O
ATOM	1012	N	ASP	A	494	5.369	16.113	15.428	1.00	27.01	A	N
ATOM	1013	CA	ASP	A	494	4.098	15.469	15.036	1.00	25.31	A	C
ATOM	1014	CB	ASP	A	494	4.385	14.448	13.959	1.00	25.40	A	C
ATOM	1015	CG	ASP	A	494	3.169	14.112	13.123	1.00	27.37	A	C
ATOM	1016	OD1	ASP	A	494	2.035	14.665	13.335	1.00	26.20	A	O
ATOM	1017	OD2	ASP	A	494	3.272	13.300	12.165	1.00	27.51	A	O
ATOM	1018	C	ASP	A	494	3.499	14.776	16.270	1.00	23.65	A	C
ATOM	1019	O	ASP	A	494	3.069	13.625	16.211	1.00	20.55	A	O
ATOM	1020	N	LEU	A	495	3.528	15.448	17.408	1.00	22.63	A	N
ATOM	1021	CA	LEU	A	495	3.214	14.759	18.629	1.00	22.90	A	C
ATOM	1022	CB	LEU	A	495	3.966	15.399	19.781	1.00	22.63	A	C
ATOM	1023	CG	LEU	A	495	3.538	14.818	21.140	1.00	25.32	A	C
ATOM	1024	CD1	LEU	A	495	3.898	13.380	21.315	1.00	20.28	A	C
ATOM	1025	CD2	LEU	A	495	4.065	15.595	22.360	1.00	26.01	A	C
ATOM	1026	C	LEU	A	495	1.709	14.793	18.778	1.00	22.95	A	C
ATOM	1027	O	LEU	A	495	1.080	15.841	18.903	1.00	23.83	A	O
ATOM	1028	N	ALA	A	496	1.109	13.642	18.787	1.00	21.60	A	N
ATOM	1029	CA	ALA	A	496	-0.342	13.542	18.652	1.00	22.22	A	C
ATOM	1030	CB	ALA	A	496	-0.724	13.730	17.041	1.00	21.08	A	C
ATOM	1031	C	ALA	A	496	-0.784	12.177	19.055	1.00	21.35	A	C
ATOM	1032	O	ALA	A	496	0.010	11.320	18.952	1.00	22.21	A	O
ATOM	1033	N	ALA	A	497	-2.043	11.926	19.364	1.00	20.75	A	N
ATOM	1034	CA	ALA	A	497	-2.431	10.553	19.791	1.00	22.98	A	C
ATOM	1035	CB	ALA	A	497	-3.879	10.487	20.217	1.00	21.60	A	C
ATOM	1036	C	ALA	A	497	-2.205	9.511	18.748	1.00	24.99	A	C
ATOM	1037	O	ALA	A	497	-1.828	8.403	19.087	1.00	26.21	A	O
ATOM	1038	N	ARG	A	498	-2.463	9.803	17.472	1.00	26.52	A	N
ATOM	1039	CA	ARG	A	498	-2.196	8.726	16.505	1.00	27.68	A	C
ATOM	1040	CB	ARG	A	498	-2.445	9.128	15.090	1.00	27.91	A	C
ATOM	1041	CG	ARG	A	498	-1.562	10.385	14.758	1.00	27.76	A	C
ATOM	1042	CD	ARG	A	498	-2.157	11.159	13.564	1.00	25.34	A	C
ATOM	1043	NE	ARG	A	498	-1.348	12.360	13.416	1.00	25.15	A	N
ATOM	1044	CZ	ARG	A	498	-1.753	13.550	13.753	1.00	21.37	A	C
ATOM	1045	NH1	ARG	A	498	-2.957	13.661	14.181	1.00	25.68	A	N
ATOM	1046	NH2	ARG	A	498	-1.011	14.619	13.573	1.00	19.80	A	N
ATOM	1047	C	ARG	A	498	-0.769	8.263	16.574	1.00	27.14	A	C
ATOM	1048	O	ARG	A	498	-0.542	7.184	16.255	1.00	27.46	A	O
ATOM	1049	N	ASN	A	499	0.173	9.089	16.985	1.00	26.64	A	N
ATOM	1050	CA	ASN	A	499	1.533	8.701	17.117	1.00	25.52	A	C
ATOM	1051	CB	ASN	A	499	2.408	9.797	16.594	1.00	23.85	A	C
ATOM	1052	CG	ASN	A	499	2.200	9.978	15.076	1.00	23.38	A	C
ATOM	1053	OD1	ASN	A	499	1.819	9.045	14.403	1.00	21.21	A	O

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ATOM	1054	ND2	ASN	A	499	2.341	11.201	14.578	1.00	17.03	A	N
ATOM	1055	C	ASN	A	499	1.965	8.241	18.531	1.00	25.60	A	C
ATOM	1056	O	ASN	A	499	3.108	8.377	18.948	1.00	23.04	A	O
ATOM	1057	N	VAL	A	500	1.040	7.749	19.289	1.00	23.79	A	N
ATOM	1058	CA	VAL	A	500	1.512	7.100	20.470	1.00	24.81	A	C
ATOM	1059	CB	VAL	A	500	0.848	7.677	21.742	1.00	25.12	A	C
ATOM	1060	CG1	VAL	A	500	1.325	6.930	22.903	1.00	23.66	A	C
ATOM	1061	CG2	VAL	A	500	1.160	9.154	21.898	1.00	23.59	A	C
ATOM	1062	C	VAL	A	500	1.098	5.681	20.318	1.00	24.49	A	C
ATOM	1063	O	VAL	A	500	-0.039	5.396	19.948	1.00	24.74	A	O
ATOM	1064	N	LEU	A	501	2.013	4.755	20.477	1.00	24.77	A	N
ATOM	1065	CA	LEU	A	501	1.629	3.361	20.271	1.00	25.24	A	C
ATOM	1066	CB	LEU	A	501	2.585	2.706	19.320	1.00	24.47	A	C
ATOM	1067	CG	LEU	A	501	2.697	3.378	17.910	1.00	25.19	A	C
ATOM	1068	CD1	LEU	A	501	3.454	2.578	16.743	1.00	23.80	A	C
ATOM	1069	CD2	LEU	A	501	1.313	3.783	17.438	1.00	25.36	A	C
ATOM	1070	C	LEU	A	501	1.647	2.684	21.576	1.00	26.95	A	C
ATOM	1071	O	LEU	A	501	2.511	2.976	22.475	1.00	24.84	A	O
ATOM	1072	N	LEU	A	502	0.671	1.771	21.720	1.00	29.21	A	N
ATOM	1073	CA	LEU	A	502	0.611	0.906	22.946	1.00	29.97	A	C
ATOM	1074	CB	LEU	A	502	-0.833	0.665	23.467	1.00	30.09	A	C
ATOM	1075	CG	LEU	A	502	-1.525	2.004	23.820	1.00	33.76	A	C
ATOM	1076	CD1	LEU	A	502	-2.948	1.834	24.422	1.00	34.24	A	C
ATOM	1077	CD2	LEU	A	502	-0.752	2.907	24.745	1.00	29.68	A	C
ATOM	1078	C	LEU	A	502	1.408	-0.399	22.894	1.00	29.52	A	C
ATOM	1079	O	LEU	A	502	1.292	-1.244	22.008	1.00	28.92	A	O
ATOM	1080	N	VAL	A	503	2.259	-0.551	23.871	1.00	30.04	A	N
ATOM	1081	CA	VAL	A	503	2.930	-1.817	24.001	1.00	31.98	A	C
ATOM	1082	CB	VAL	A	503	4.276	-1.626	24.620	1.00	32.41	A	C
ATOM	1083	CG1	VAL	A	503	4.952	-2.887	24.788	1.00	34.96	A	C
ATOM	1084	CG2	VAL	A	503	5.081	-0.759	23.768	1.00	32.76	A	C
ATOM	1085	C	VAL	A	503	1.995	-2.795	24.797	1.00	30.69	A	C
ATOM	1086	O	VAL	A	503	1.818	-3.911	24.411	1.00	29.65	A	O
ATOM	1087	N	THR	A	504	1.437	-2.319	25.872	1.00	28.62	A	N
ATOM	1088	CA	THR	A	504	0.463	-2.983	26.615	1.00	28.57	A	C
ATOM	1089	CB	THR	A	504	1.017	-3.488	27.929	1.00	29.52	A	C
ATOM	1090	OG1	THR	A	504	1.258	-2.396	28.885	1.00	28.60	A	O
ATOM	1091	CG2	THR	A	504	2.232	-4.278	27.786	1.00	29.57	A	C
ATOM	1092	C	THR	A	504	-0.562	-1.874	27.023	1.00	29.07	A	C
ATOM	1093	O	THR	A	504	-0.368	-0.685	26.858	1.00	27.80	A	O
ATOM	1094	N	GLN	A	505	-1.655	-2.284	27.613	1.00	29.00	A	N
ATOM	1095	CA	GLN	A	505	-2.619	-1.378	28.130	1.00	30.29	A	C
ATOM	1096	CB	GLN	A	505	-3.702	-2.261	28.733	1.00	31.82	A	C
ATOM	1097	CG	AGLN	A	505	-4.412	-3.297	27.806	0.70	33.59	A	C
ATOM	1098	CG	BGLN	A	505	-4.391	-3.272	27.811	0.30	32.98	A	C
ATOM	1099	CD	AGLN	A	505	-3.720	-4.762	27.588	0.70	35.34	A	C
ATOM	1100	CD	BGLN	A	505	-4.016	-4.760	28.079	0.30	34.78	A	C
ATOM	1101	OE1AGLN	A	505	-2.503	-4.990	27.901	0.70	34.99	A	O	
ATOM	1102	OE1BGLN	A	505	-2.811	-5.126	28.133	0.30	35.17	A	O	
ATOM	1103	NE2AGLN	A	505	-4.542	-5.726	27.013	0.70	32.62	A	N	
ATOM	1104	NE2BGLN	A	505	-5.053	-5.619	28.231	0.30	33.71	A	N	
ATOM	1105	C	GLN	A	505	-2.005	-0.412	29.231	1.00	29.32	A	C
ATOM	1106	O	GLN	A	505	-2.587	0.588	29.549	1.00	29.86	A	O
ATOM	1107	N	HIS	A	506	-0.804	-0.678	29.752	1.00	26.76	A	N
ATOM	1108	CA	HIS	A	506	-0.188	0.217	30.710	1.00	26.15	A	C
ATOM	1109	CB	HIS	A	506	-0.087	-0.540	32.053	1.00	26.55	A	C
ATOM	1110	CG	HIS	A	506	-1.422	-0.705	32.694	1.00	27.95	A	C
ATOM	1111	ND1	HIS	A	506	-2.125	0.357	33.203	1.00	30.32	A	N
ATOM	1112	CE1	HIS	A	506	-3.284	-0.062	33.673	1.00	33.32	A	C
ATOM	1113	NE2	HIS	A	506	-3.350	-1.369	33.500	1.00	32.87	A	N
ATOM	1114	CD2	HIS	A	506	-2.245	-1.779	32.804	1.00	30.67	A	C
ATOM	1115	C	HIS	A	506	1.238	0.724	30.325	1.00	25.45	A	C

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ATOM	1116	O	HIS	A	506	2.075	1.044	31.213	1.00	21.22	A	O
ATOM	1117	N	TYR	A	507	1.529	0.691	29.018	1.00	24.28	A	N
ATOM	1118	CA	TYR	A	507	2.837	1.071	28.540	1.00	25.45	A	C
ATOM	1119	CB	TYR	A	507	3.776	-0.197	28.539	1.00	26.22	A	C
ATOM	1120	CG	TYR	A	507	5.284	-0.019	28.232	1.00	28.13	A	C
ATOM	1121	CD1	TYR	A	507	5.825	1.247	27.903	1.00	30.52	A	C
ATOM	1122	CE1	TYR	A	507	7.180	1.423	27.650	1.00	24.69	A	C
ATOM	1123	CZ	TYR	A	507	8.039	0.352	27.657	1.00	29.16	A	C
ATOM	1124	OH	TYR	A	507	9.405	0.598	27.316	1.00	29.20	A	O
ATOM	1125	CE2	TYR	A	507	7.550	-0.921	28.021	1.00	27.03	A	C
ATOM	1126	CD2	TYR	A	507	6.179	-1.089	28.268	1.00	25.65	A	C
ATOM	1127	C	TYR	A	507	2.744	1.716	27.163	1.00	25.30	A	C
ATOM	1128	O	TYR	A	507	2.517	1.011	26.102	1.00	23.20	A	O
ATOM	1129	N	ALA	A	508	2.954	3.033	27.151	1.00	23.73	A	N
ATOM	1130	CA	ALA	A	508	2.837	3.795	25.933	1.00	22.95	A	C
ATOM	1131	CB	ALA	A	508	2.065	5.050	26.280	1.00	20.82	A	C
ATOM	1132	C	ALA	A	508	4.166	4.211	25.323	1.00	23.81	A	C
ATOM	1133	O	ALA	A	508	5.093	4.524	26.036	1.00	24.90	A	O
ATOM	1134	N	LYS	A	509	4.267	4.381	24.013	1.00	24.69	A	N
ATOM	1135	CA	LYS	A	509	5.560	4.840	23.451	1.00	25.36	A	C
ATOM	1136	CB	LYS	A	509	6.288	3.689	22.714	1.00	25.38	A	C
ATOM	1137	CG	LYS	A	509	7.369	2.976	23.478	1.00	26.70	A	C
ATOM	1138	CD	LYS	A	509	7.584	1.537	23.018	1.00	30.86	A	C
ATOM	1139	CE	LYS	A	509	7.988	0.688	24.198	1.00	33.98	A	C
ATOM	1140	NZ	LYS	A	509	9.416	0.820	24.416	1.00	34.97	A	N
ATOM	1141	C	LYS	A	509	5.365	5.859	22.403	1.00	24.95	A	C
ATOM	1142	O	LYS	A	509	4.421	5.738	21.672	1.00	25.98	A	O
ATOM	1143	N	ILE	A	510	6.296	6.780	22.208	1.00	24.17	A	N
ATOM	1144	CA	ILE	A	510	6.091	7.800	21.188	1.00	24.81	A	C
ATOM	1145	CB	ILE	A	510	6.879	9.088	21.668	1.00	25.45	A	C
ATOM	1146	CG1	ILE	A	510	6.208	9.589	22.919	1.00	23.72	A	C
ATOM	1147	CD1	ILE	A	510	7.053	10.583	23.648	1.00	26.20	A	C
ATOM	1148	CG2	ILE	A	510	7.028	10.201	20.576	1.00	19.18	A	C
ATOM	1149	C	ILE	A	510	6.652	7.359	19.857	1.00	25.93	A	C
ATOM	1150	O	ILE	A	510	7.765	6.842	19.769	1.00	26.11	A	O
ATOM	1151	N	SER	A	511	5.927	7.476	18.797	1.00	26.01	A	N
ATOM	1152	CA	SER	A	511	6.552	7.061	17.551	1.00	26.14	A	C
ATOM	1153	CB	SER	A	511	5.830	5.910	16.971	1.00	26.88	A	C
ATOM	1154	OG	SER	A	511	4.623	6.463	16.492	1.00	33.47	A	O
ATOM	1155	C	SER	A	511	6.441	8.163	16.562	1.00	25.76	A	C
ATOM	1156	O	SER	A	511	5.899	9.222	16.888	1.00	23.16	A	O
ATOM	1157	N	ASP	A	512	6.875	7.850	15.329	1.00	25.82	A	N
ATOM	1158	CA	ASP	A	512	6.860	8.654	14.173	1.00	25.80	A	C
ATOM	1159	CB	ASP	A	512	5.502	8.914	13.691	1.00	27.80	A	C
ATOM	1160	CG	ASP	A	512	5.504	9.446	12.279	1.00	30.10	A	C
ATOM	1161	OD1	ASP	A	512	6.608	9.734	11.697	1.00	28.36	A	O
ATOM	1162	OD2	ASP	A	512	4.421	9.629	11.704	1.00	30.86	A	O
ATOM	1163	C	ASP	A	512	7.619	9.940	14.215	1.00	26.35	A	C
ATOM	1164	O	ASP	A	512	7.060	11.044	14.374	1.00	23.43	A	O
ATOM	1165	N	PHE	A	513	8.890	9.760	13.887	1.00	27.09	A	N
ATOM	1166	CA	PHE	A	513	9.843	10.762	13.776	1.00	27.42	A	C
ATOM	1167	CB	PHE	A	513	11.115	10.266	14.383	1.00	25.93	A	C
ATOM	1168	CG	PHE	A	513	10.973	10.036	15.863	1.00	27.55	A	C
ATOM	1169	CD1	PHE	A	513	10.568	8.800	16.352	1.00	29.82	A	C
ATOM	1170	CE1	PHE	A	513	10.342	8.588	17.712	1.00	28.61	A	C
ATOM	1171	CZ	PHE	A	513	10.507	9.580	18.583	1.00	28.80	A	C
ATOM	1172	CE2	PHE	A	513	10.949	10.792	18.113	1.00	31.20	A	C
ATOM	1173	CD2	PHE	A	513	11.126	11.038	16.755	1.00	27.40	A	C
ATOM	1174	C	PHE	A	513	9.962	11.335	12.348	1.00	27.72	A	C
ATOM	1175	O	PHE	A	513	10.774	12.180	12.145	1.00	28.64	A	O
ATOM	1176	N	GLY	A	514	9.150	10.928	11.394	1.00	26.61	A	N
ATOM	1177	CA	GLY	A	514	9.164	11.618	10.120	1.00	28.35	A	C

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Figure 2A - 20

ATOM	1178	C	GLY	A	514	9.377	13.151	9.902	1.00	30.09	A	C
ATOM	1179	O	GLY	A	514	9.856	13.571	8.857	1.00	31.25	A	O
ATOM	1180	N	LEU	A	515	8.972	13.985	10.842	1.00	29.34	A	N
ATOM	1181	CA	LEU	A	515	9.193	15.388	10.771	1.00	28.26	A	C
ATOM	1182	CB	LEU	A	515	7.873	16.130	11.034	1.00	28.56	A	C
ATOM	1183	CG	LEU	A	515	6.848	16.017	9.896	1.00	32.77	A	C
ATOM	1184	CD1	LEU	A	515	5.424	16.253	10.223	1.00	34.35	A	C
ATOM	1185	CD2	LEU	A	515	7.206	16.918	8.801	1.00	35.46	A	C
ATOM	1186	C	LEU	A	515	10.180	15.771	11.870	1.00	28.15	A	C
ATOM	1187	O	LEU	A	515	10.434	16.994	12.064	1.00	26.59	A	O
ATOM	1188	N	SER	A	516	10.725	14.837	12.644	1.00	26.11	A	N
ATOM	1189	CA	SER	A	516	11.566	15.442	13.639	1.00	30.82	A	C
ATOM	1190	CB	SER	A	516	11.710	14.618	14.948	1.00	32.27	A	C
ATOM	1191	OG	SER	A	516	11.932	13.258	14.626	1.00	38.10	A	O
ATOM	1192	C	SER	A	516	12.909	16.033	13.185	1.00	30.23	A	C
ATOM	1193	O	SER	A	516	13.324	15.941	12.004	1.00	29.91	A	O
ATOM	1194	N	LYS	A	517	13.541	16.699	14.138	1.00	28.73	A	N
ATOM	1195	CA	LYS	A	517	14.756	17.466	13.860	1.00	27.45	A	C
ATOM	1196	CB	LYS	A	517	14.476	18.919	13.497	1.00	24.22	A	C
ATOM	1197	CG	LYS	A	517	13.633	19.130	12.328	1.00	24.04	A	C
ATOM	1198	CD	LYS	A	517	14.149	18.431	11.001	1.00	26.64	A	C
ATOM	1199	CE	LYS	A	517	13.236	18.936	9.833	1.00	30.84	A	C
ATOM	1200	NZ	LYS	A	517	13.543	18.420	8.406	1.00	33.29	A	N
ATOM	1201	C	LYS	A	517	15.573	17.544	15.106	1.00	29.19	A	C
ATOM	1202	O	LYS	A	517	15.032	17.798	16.287	1.00	28.19	A	O
ATOM	1203	N	ALA	A	518	16.880	17.368	14.861	1.00	28.67	A	N
ATOM	1204	CA	ALA	A	518	17.821	17.600	15.926	1.00	29.26	A	C
ATOM	1205	CB	ALA	A	518	19.065	16.691	15.702	1.00	30.18	A	C
ATOM	1206	C	ALA	A	518	18.207	19.073	15.800	1.00	29.23	A	C
ATOM	1207	O	ALA	A	518	18.438	19.547	14.704	1.00	27.75	A	O
ATOM	1208	N	LEU	A	519	18.168	19.768	16.929	1.00	29.23	A	N
ATOM	1209	CA	LEU	A	519	18.582	21.134	17.118	1.00	30.05	A	C
ATOM	1210	CB	LEU	A	519	18.098	21.630	18.492	1.00	30.14	A	C
ATOM	1211	CG	LEU	A	519	16.525	21.719	18.807	1.00	33.91	A	C
ATOM	1212	CD1	LEU	A	519	16.173	22.631	20.021	1.00	39.59	A	C
ATOM	1213	CD2	LEU	A	519	15.587	22.212	17.684	1.00	27.61	A	C
ATOM	1214	C	LEU	A	519	20.092	21.397	17.023	1.00	31.17	A	C
ATOM	1215	O	LEU	A	519	20.938	20.648	17.525	1.00	30.74	A	O
ATOM	1216	N	ARG	A	520	20.460	22.491	16.376	1.00	31.39	A	N
ATOM	1217	CA	ARG	A	520	21.842	22.745	16.237	1.00	31.70	A	C
ATOM	1218	CB	ARG	A	520	22.016	23.846	15.181	1.00	32.05	A	C
ATOM	1219	CG	ARG	A	520	21.626	23.377	13.709	1.00	31.87	A	C
ATOM	1220	CD	ARG	A	520	21.357	24.580	12.743	1.00	30.47	A	C
ATOM	1221	NE	ARG	A	520	22.235	25.702	13.063	1.00	32.31	A	N
ATOM	1222	CZ	ARG	A	520	23.027	26.296	12.175	1.00	32.70	A	C
ATOM	1223	NH1	ARG	A	520	23.024	25.902	10.918	1.00	33.07	A	N
ATOM	1224	NH2	ARG	A	520	23.845	27.272	12.539	1.00	32.43	A	N
ATOM	1225	C	ARG	A	520	22.283	23.172	17.590	1.00	32.04	A	C
ATOM	1226	O	ARG	A	520	21.494	23.712	18.358	1.00	30.91	A	O
ATOM	1227	N	ALA	A	521	23.566	23.026	17.914	1.00	33.49	A	N
ATOM	1228	CA	ALA	A	521	23.990	23.471	19.235	1.00	33.60	A	C
ATOM	1229	CB	ALA	A	521	25.315	23.117	19.487	1.00	34.16	A	C
ATOM	1230	C	ALA	A	521	23.958	24.893	19.345	1.00	34.23	A	C
ATOM	1231	O	ALA	A	521	24.239	25.419	20.422	1.00	35.92	A	O
ATOM	1232	N	ASP	A	522	23.686	25.595	18.272	1.00	34.00	A	N
ATOM	1233	CA	ASP	A	522	23.644	27.053	18.474	1.00	34.75	A	C
ATOM	1234	CB	ASP	A	522	24.483	27.825	17.487	1.00	32.89	A	C
ATOM	1235	CG	ASP	A	522	24.077	27.577	16.059	1.00	33.91	A	C
ATOM	1236	OD1	ASP	A	522	23.293	26.625	15.702	1.00	27.49	A	O
ATOM	1237	OD2	ASP	A	522	24.575	28.322	15.171	1.00	36.53	A	O
ATOM	1238	C	ASP	A	522	22.252	27.669	18.462	1.00	35.19	A	C
ATOM	1239	O	ASP	A	522	22.168	28.903	18.329	1.00	34.55	A	O

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## Figure 2A - 21

ATOM	1240	N	GLU	A	523	21.202	26.839	18.623	1.00	35.20	A	N
ATOM	1241	CA	GLU	A	523	19.787	27.362	18.538	1.00	35.77	A	C
ATOM	1242	CB	GLU	A	523	19.241	27.260	17.135	1.00	35.09	A	C
ATOM	1243	CG	GLU	A	523	18.732	25.867	16.905	1.00	38.78	A	C
ATOM	1244	CD	GLU	A	523	18.818	25.404	15.422	1.00	42.75	A	C
ATOM	1245	OE1	GLU	A	523	18.911	26.295	14.479	1.00	40.52	A	O
ATOM	1246	OE2	GLU	A	523	18.717	24.141	15.204	1.00	44.22	A	O
ATOM	1247	C	GLU	A	523	18.807	26.660	19.446	1.00	35.09	A	C
ATOM	1248	O	GLU	A	523	19.015	25.512	19.785	1.00	33.07	A	O
ATOM	1249	N	ASN	A	524	17.736	27.328	19.852	1.00	35.64	A	N
ATOM	1250	CA	ASN	A	524	16.739	26.615	20.647	1.00	35.76	A	C
ATOM	1251	CB	ASN	A	524	16.295	27.359	21.895	1.00	37.92	A	C
ATOM	1252	CG	ASN	A	524	17.245	28.527	22.218	1.00	42.89	A	C
ATOM	1253	OD1	ASN	A	524	17.000	29.641	21.750	1.00	47.07	A	O
ATOM	1254	ND2	ASN	A	524	18.334	28.284	23.006	1.00	45.49	A	N
ATOM	1255	C	ASN	A	524	15.577	26.237	19.919	1.00	33.99	A	C
ATOM	1256	O	ASN	A	524	14.755	25.723	20.533	1.00	35.93	A	O
ATOM	1257	O1P	PTR	A	525	14.537	33.591	17.375	1.00	50.93	A	O
ATOM	1258	P	PTR	A	525	15.376	33.372	16.131	1.00	52.24	A	P
ATOM	1259	O2P	PTR	A	525	16.854	33.494	16.571	1.00	50.68	A	O
ATOM	1260	O3P	PTR	A	525	15.016	34.057	14.785	1.00	53.03	A	O
ATOM	1261	OH	PTR	A	525	15.118	31.932	15.495	1.00	48.83	A	O
ATOM	1262	CZ	PTR	A	525	14.734	30.939	16.106	1.00	43.90	A	C
ATOM	1263	CE2	PTR	A	525	14.261	29.920	15.308	1.00	41.73	A	C
ATOM	1264	CD2	PTR	A	525	13.819	28.738	15.848	1.00	40.12	A	C
ATOM	1265	CE1	PTR	A	525	14.699	30.809	17.479	1.00	41.68	A	C
ATOM	1266	CD1	PTR	A	525	14.249	29.597	18.037	1.00	40.90	A	C
ATOM	1267	CG	PTR	A	525	13.841	28.520	17.214	1.00	37.07	A	C
ATOM	1268	CB	PTR	A	525	13.352	27.190	17.786	1.00	32.92	A	C
ATOM	1269	CA	PTR	A	525	14.365	26.039	17.863	1.00	32.47	A	C
ATOM	1270	N	PTR	A	525	15.507	26.408	18.623	1.00	32.18	A	N
ATOM	1271	C	PTR	A	525	14.829	25.704	16.461	1.00	32.15	A	C
ATOM	1272	O	PTR	A	525	15.929	26.038	16.208	1.00	31.96	A	O
ATOM	1273	O1P	PTR	A	526	15.417	21.266	7.763	1.00	48.06	A	O
ATOM	1274	P	PTR	A	526	14.196	22.008	7.378	1.00	48.83	A	P
ATOM	1275	O2P	PTR	A	526	13.616	21.226	6.202	1.00	50.70	A	O
ATOM	1276	O3P	PTR	A	526	14.421	23.503	7.136	1.00	46.92	A	O
ATOM	1277	OH	PTR	A	526	13.197	22.084	8.632	1.00	43.54	A	O
ATOM	1278	CZ	PTR	A	526	13.510	22.414	9.802	1.00	34.76	A	C
ATOM	1279	CE2	PTR	A	526	12.425	22.552	10.645	1.00	31.00	A	C
ATOM	1280	CD2	PTR	A	526	12.608	22.818	12.000	1.00	29.03	A	C
ATOM	1281	CE1	PTR	A	526	14.801	22.576	10.298	1.00	29.79	A	C
ATOM	1282	CD1	PTR	A	526	14.995	22.845	11.649	1.00	30.90	A	C
ATOM	1283	CG	PTR	A	526	13.849	22.999	12.536	1.00	32.82	A	C
ATOM	1284	CB	PTR	A	526	13.987	23.334	14.024	1.00	33.76	A	C
ATOM	1285	CA	PTR	A	526	14.418	24.782	14.282	1.00	33.30	A	C
ATOM	1286	N	PTR	A	526	14.048	25.043	15.622	1.00	31.50	A	N
ATOM	1287	C	PTR	A	526	13.487	25.546	13.415	1.00	35.61	A	C
ATOM	1288	O	PTR	A	526	12.273	25.462	13.470	1.00	34.63	A	O
ATOM	1289	N	LYS	A	527	14.031	26.346	12.547	1.00	39.16	A	N
ATOM	1290	CA	LYS	A	527	13.136	27.202	11.758	1.00	41.36	A	C
ATOM	1291	CB	LYS	A	527	13.724	28.606	11.543	1.00	42.40	A	C
ATOM	1292	CG	LYS	A	527	12.686	29.727	11.085	1.00	46.01	A	C
ATOM	1293	CD	LYS	A	527	12.243	29.557	9.567	1.00	46.13	A	C
ATOM	1294	CE	LYS	A	527	12.189	30.861	8.778	1.00	47.67	A	C
ATOM	1295	NZ	LYS	A	527	12.346	30.669	7.249	1.00	48.28	A	N
ATOM	1296	C	LYS	A	527	12.947	26.527	10.482	1.00	41.54	A	C
ATOM	1297	O	LYS	A	527	13.851	26.254	9.832	1.00	44.25	A	O
ATOM	1298	N	ALA	A	528	11.748	26.261	10.117	1.00	42.46	A	N
ATOM	1299	CA	ALA	A	528	11.453	25.579	8.916	1.00	44.80	A	C
ATOM	1300	CB	ALA	A	528	10.045	24.995	9.093	1.00	44.63	A	C
ATOM	1301	C	ALA	A	528	11.459	26.515	7.749	1.00	46.21	A	C

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## Figure 2A - 22

ATOM	1302	O	ALA	A	528	11.380	27.680	7.894	1.00	45.54	A	O
ATOM	1303	N	GLN	A	529	11.520	25.989	6.565	1.00	49.91	A	N
ATOM	1304	CA	GLN	A	529	11.487	26.842	5.373	1.00	54.77	A	C
ATOM	1305	CB	GLN	A	529	12.788	26.721	4.564	1.00	55.86	A	C
ATOM	1306	CG	GLN	A	529	14.021	26.616	5.426	1.00	58.36	A	C
ATOM	1307	CD	GLN	A	529	14.754	27.991	5.587	1.00	60.87	A	C
ATOM	1308	OE1	GLN	A	529	14.258	29.064	5.086	1.00	58.37	A	O
ATOM	1309	NE2	GLN	A	529	15.967	27.943	6.235	1.00	59.36	A	N
ATOM	1310	C	GLN	A	529	10.428	26.295	4.478	1.00	56.71	A	C
ATOM	1311	O	GLN	A	529	10.777	25.415	3.636	1.00	55.42	A	O
ATOM	1312	N	THR	A	530	9.188	26.807	4.706	1.00	59.29	A	N
ATOM	1313	CA	THR	A	530	7.906	26.492	4.033	1.00	61.59	A	C
ATOM	1314	CB	THR	A	530	7.926	26.654	2.446	1.00	62.48	A	C
ATOM	1315	OG1	THR	A	530	6.609	26.370	1.922	1.00	64.96	A	O
ATOM	1316	CG2	THR	A	530	8.836	25.613	1.760	1.00	62.14	A	C
ATOM	1317	C	THR	A	530	7.082	25.241	4.483	1.00	62.75	A	C
ATOM	1318	O	THR	A	530	7.555	24.055	4.614	1.00	63.33	A	O
ATOM	1319	N	HIS	A	531	5.830	25.585	4.738	1.00	62.53	A	N
ATOM	1320	CA	HIS	A	531	4.772	24.709	5.107	1.00	62.59	A	C
ATOM	1321	CB	HIS	A	531	3.540	25.542	4.818	1.00	63.98	A	C
ATOM	1322	CG	HIS	A	531	2.418	25.296	5.753	1.00	65.54	A	C
ATOM	1323	ND1	HIS	A	531	1.885	24.041	5.940	1.00	67.34	A	N
ATOM	1324	CE1	HIS	A	531	0.878	24.125	6.791	1.00	66.89	A	C
ATOM	1325	NE2	HIS	A	531	0.752	25.388	7.169	1.00	66.76	A	N
ATOM	1326	CD2	HIS	A	531	1.709	26.137	6.540	1.00	66.09	A	C
ATOM	1327	C	HIS	A	531	4.748	23.482	4.193	1.00	61.98	A	C
ATOM	1328	O	HIS	A	531	4.514	23.606	2.936	1.00	61.86	A	O
ATOM	1329	N	GLY	A	532	4.994	22.304	4.789	1.00	60.39	A	N
ATOM	1330	CA	GLY	A	532	4.964	21.054	4.045	1.00	56.81	A	C
ATOM	1331	C	GLY	A	532	3.816	20.094	4.454	1.00	54.54	A	C
ATOM	1332	O	GLY	A	532	4.039	18.910	4.824	1.00	55.93	A	O
ATOM	1333	N	LYS	A	533	2.569	20.498	4.433	1.00	49.64	A	N
ATOM	1334	CA	LYS	A	533	1.658	19.397	4.739	1.00	45.84	A	C
ATOM	1335	CB	LYS	A	533	2.122	18.171	3.944	1.00	46.40	A	C
ATOM	1336	CG	LYS	A	533	3.521	17.638	3.879	0.00	8.00	A	C
ATOM	1337	CD	LYS	A	533	3.770	17.057	2.475	0.00	8.00	A	C
ATOM	1338	CE	LYS	A	533	5.243	17.057	2.047	0.00	8.00	A	C
ATOM	1339	NZ	LYS	A	533	6.091	16.642	3.159	0.00	8.00	A	N
ATOM	1340	C	LYS	A	533	1.859	19.114	6.217	1.00	41.85	A	C
ATOM	1341	O	LYS	A	533	2.688	18.259	6.610	1.00	41.34	A	O
ATOM	1342	N	TRP	A	534	1.136	19.852	7.028	1.00	37.65	A	N
ATOM	1343	CA	TRP	A	534	1.473	19.938	8.461	1.00	33.76	A	C
ATOM	1344	CB	TRP	A	534	1.963	21.352	8.841	1.00	32.84	A	C
ATOM	1345	CG	TRP	A	534	3.439	21.677	8.639	1.00	30.43	A	C
ATOM	1346	CD1	TRP	A	534	4.429	20.816	8.155	1.00	30.48	A	C
ATOM	1347	NE1	TRP	A	534	5.629	21.505	8.069	1.00	30.18	A	N
ATOM	1348	CE2	TRP	A	534	5.457	22.807	8.477	1.00	28.92	A	C
ATOM	1349	CD2	TRP	A	534	4.087	22.967	8.823	1.00	26.24	A	C
ATOM	1350	CE3	TRP	A	534	3.658	24.240	9.279	1.00	23.45	A	C
ATOM	1351	CZ3	TRP	A	534	4.649	25.324	9.404	1.00	19.56	A	C
ATOM	1352	CH2	TRP	A	534	5.993	25.082	9.035	1.00	23.34	A	C
ATOM	1353	CZ2	TRP	A	534	6.416	23.860	8.598	1.00	26.17	A	C
ATOM	1354	C	TRP	A	534	0.261	19.584	9.246	1.00	30.94	A	C
ATOM	1355	O	TRP	A	534	-0.844	19.784	8.794	1.00	29.23	A	O
ATOM	1356	N	PRO	A	535	0.456	18.991	10.396	1.00	29.53	A	N
ATOM	1357	CA	PRO	A	535	-0.681	18.715	11.285	1.00	28.96	A	C
ATOM	1358	CB	PRO	A	535	-0.156	17.661	12.198	1.00	29.03	A	C
ATOM	1359	CG	PRO	A	535	1.522	17.999	12.252	1.00	29.20	A	C
ATOM	1360	CD	PRO	A	535	1.753	18.619	10.963	1.00	29.53	A	C
ATOM	1361	C	PRO	A	535	-1.068	20.005	12.055	1.00	28.41	A	C
ATOM	1362	O	PRO	A	535	-0.950	20.085	13.277	1.00	29.19	A	O
ATOM	1363	N	VAL	A	536	-1.594	20.989	11.337	1.00	26.55	A	N

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Figure 2A - 23

ATOM	1364	CA	VAL	A	536	-1.919	22.231	11.953	1.00	26.04	A	C
ATOM	1365	CB	VAL	A	536	-2.554	23.133	10.940	1.00	25.58	A	C
ATOM	1366	CG1	VAL	A	536	-1.435	23.520	9.893	1.00	23.24	A	C
ATOM	1367	CG2	VAL	A	536	-3.647	22.394	10.307	1.00	21.03	A	C
ATOM	1368	C	VAL	A	536	-2.699	22.224	13.234	1.00	26.61	A	C
ATOM	1369	O	VAL	A	536	-2.434	22.991	14.005	1.00	26.04	A	O
ATOM	1370	N	LYS	A	537	-3.657	21.335	13.445	1.00	28.72	A	N
ATOM	1371	CA	LYS	A	537	-4.477	21.351	14.671	1.00	29.00	A	C
ATOM	1372	CB	LYS	A	537	-5.641	20.351	14.544	1.00	30.38	A	C
ATOM	1373	CG	LYS	A	537	-6.860	20.871	13.821	1.00	29.45	A	C
ATOM	1374	CD	LYS	A	537	-7.595	19.826	13.106	1.00	27.48	A	C
ATOM	1375	CE	LYS	A	537	-8.730	20.559	12.511	1.00	32.09	A	C
ATOM	1376	NZ	LYS	A	537	-9.590	19.704	11.733	1.00	37.57	A	N
ATOM	1377	C	LYS	A	537	-3.641	20.994	15.868	1.00	26.60	A	C
ATOM	1378	O	LYS	A	537	-4.083	21.146	17.010	1.00	24.10	A	O
ATOM	1379	N	TRP	A	538	-2.428	20.534	15.621	1.00	24.64	A	N
ATOM	1380	CA	TRP	A	538	-1.572	20.262	16.787	1.00	24.75	A	C
ATOM	1381	CB	TRP	A	538	-0.963	18.884	16.701	1.00	24.22	A	C
ATOM	1382	CG	TRP	A	538	-1.913	17.714	16.986	1.00	24.60	A	C
ATOM	1383	CD1	TRP	A	538	-1.934	16.994	18.088	1.00	24.10	A	C
ATOM	1384	NE1	TRP	A	538	-2.865	15.996	17.977	1.00	28.36	A	N
ATOM	1385	CE2	TRP	A	538	-3.468	16.100	16.763	1.00	27.56	A	C
ATOM	1386	CD2	TRP	A	538	-2.880	17.173	16.119	1.00	25.37	A	C
ATOM	1387	CE3	TRP	A	538	-3.292	17.479	14.827	1.00	27.09	A	C
ATOM	1388	CZ3	TRP	A	538	-4.290	16.747	14.258	1.00	25.96	A	C
ATOM	1389	CH2	TRP	A	538	-4.879	15.652	14.943	1.00	23.81	A	C
ATOM	1390	CZ2	TRP	A	538	-4.504	15.346	16.211	1.00	25.96	A	C
ATOM	1391	C	TRP	A	538	-0.406	21.195	16.980	1.00	24.87	A	C
ATOM	1392	O	TRP	A	538	0.494	20.948	17.806	1.00	26.78	A	O
ATOM	1393	N	TYR	A	539	-0.409	22.274	16.267	1.00	24.08	A	N
ATOM	1394	CA	TYR	A	539	0.743	23.173	16.228	1.00	26.49	A	C
ATOM	1395	CB	TYR	A	539	1.118	23.472	14.769	1.00	24.69	A	C
ATOM	1396	CG	TYR	A	539	2.037	22.509	14.095	1.00	27.22	A	C
ATOM	1397	CD1	TYR	A	539	2.554	21.435	14.765	1.00	28.93	A	C
ATOM	1398	CE1	TYR	A	539	3.408	20.592	14.137	1.00	30.15	A	C
ATOM	1399	CZ	TYR	A	539	3.741	20.779	12.780	1.00	28.41	A	C
ATOM	1400	OH	TYR	A	539	4.572	19.862	12.190	1.00	26.01	A	O
ATOM	1401	CE2	TYR	A	539	3.247	21.786	12.095	1.00	25.86	A	C
ATOM	1402	CD2	TYR	A	539	2.410	22.671	12.745	1.00	27.93	A	C
ATOM	1403	C	TYR	A	539	0.482	24.486	17.010	1.00	27.41	A	C
ATOM	1404	O	TYR	A	539	-0.632	24.964	17.028	1.00	27.89	A	O
ATOM	1405	N	ALA	A	540	1.495	24.954	17.757	1.00	27.08	A	N
ATOM	1406	CA	ALA	A	540	1.481	26.205	18.457	1.00	26.83	A	C
ATOM	1407	CB	ALA	A	540	2.729	26.300	19.392	1.00	26.31	A	C
ATOM	1408	C	ALA	A	540	1.435	27.424	17.517	1.00	27.14	A	C
ATOM	1409	O	ALA	A	540	1.944	27.360	16.442	1.00	26.90	A	O
ATOM	1410	N	PRO	A	541	0.905	28.556	17.954	1.00	27.79	A	N
ATOM	1411	CA	PRO	A	541	0.872	29.748	17.095	1.00	28.57	A	C
ATOM	1412	CB	PRO	A	541	0.408	30.880	18.011	1.00	28.82	A	C
ATOM	1413	CG	PRO	A	541	0.053	30.151	19.345	1.00	27.57	A	C
ATOM	1414	CD	PRO	A	541	0.441	28.804	19.313	1.00	26.95	A	C
ATOM	1415	C	PRO	A	541	2.274	30.073	16.680	1.00	27.66	A	C
ATOM	1416	O	PRO	A	541	2.352	30.556	15.602	1.00	26.88	A	O
ATOM	1417	N	GLU	A	542	3.336	29.901	17.467	1.00	26.42	A	N
ATOM	1418	CA	GLU	A	542	4.618	30.220	16.844	1.00	26.87	A	C
ATOM	1419	CB	GLU	A	542	5.725	30.103	17.846	1.00	27.36	A	C
ATOM	1420	CG	GLU	A	542	5.948	28.621	18.144	1.00	28.85	A	C
ATOM	1421	CD	GLU	A	542	5.357	28.244	19.513	1.00	27.78	A	C
ATOM	1422	OE1	GLU	A	542	4.499	29.004	20.104	1.00	21.75	A	O
ATOM	1423	OE2	GLU	A	542	5.738	27.166	19.950	1.00	24.29	A	O
ATOM	1424	C	GLU	A	542	5.051	29.422	15.521	1.00	25.82	A	C
ATOM	1425	O	GLU	A	542	5.862	29.908	14.788	1.00	22.08	A	O

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## Figure 2A - 24

ATOM	1426	N	CYS A 543	4.563	28.207	15.327	1.00	25.87	A	N
ATOM	1427	CA	CYS A 543	4.897	27.301	14.250	1.00	27.20	A	C
ATOM	1428	CB	CYS A 543	4.401	25.835	14.586	1.00	26.45	A	C
ATOM	1429	SG	CYS A 543	4.893	25.261	16.334	1.00	29.10	A	S
ATOM	1430	C	CYS A 543	4.146	27.731	13.039	1.00	29.99	A	C
ATOM	1431	O	CYS A 543	4.695	27.693	11.910	1.00	29.31	A	O
ATOM	1432	N	ILE A 544	2.863	28.066	13.227	1.00	31.07	A	N
ATOM	1433	CA	ILE A 544	1.989	28.441	12.123	1.00	32.30	A	C
ATOM	1434	CB	ILE A 544	0.504	28.504	12.657	1.00	32.88	A	C
ATOM	1435	CG1	ILE A 544	0.030	27.072	13.110	1.00	35.52	A	C
ATOM	1436	CD1	ILE A 544	0.347	25.978	12.009	1.00	33.03	A	C
ATOM	1437	CG2	ILE A 544	-0.505	28.991	11.717	1.00	27.52	A	C
ATOM	1438	C	ILE A 544	2.350	29.831	11.693	1.00	34.13	A	C
ATOM	1439	O	ILE A 544	2.325	30.113	10.515	1.00	34.56	A	O
ATOM	1440	N	ASN A 545	2.681	30.717	12.623	1.00	35.38	A	N
ATOM	1441	CA	ASN A 545	2.948	32.086	12.255	1.00	36.93	A	C
ATOM	1442	CB	ASN A 545	2.462	33.006	13.334	1.00	36.49	A	C
ATOM	1443	CG	ASN A 545	0.964	33.065	13.370	1.00	38.23	A	C
ATOM	1444	OD1	ASN A 545	0.326	33.217	14.448	1.00	33.37	A	O
ATOM	1445	ND2	ASN A 545	0.370	32.982	12.156	1.00	39.13	A	N
ATOM	1446	C	ASN A 545	4.385	32.452	11.918	1.00	38.41	A	C
ATOM	1447	O	ASN A 545	4.641	33.496	11.259	1.00	39.10	A	O
ATOM	1448	N	TYR A 546	5.312	31.641	12.424	1.00	37.34	A	N
ATOM	1449	CA	TYR A 546	6.743	31.924	12.284	1.00	36.25	A	C
ATOM	1450	CB	TYR A 546	7.278	32.545	13.598	1.00	37.50	A	C
ATOM	1451	CG	TYR A 546	6.554	33.808	13.931	1.00	42.31	A	C
ATOM	1452	CD1	TYR A 546	6.923	34.990	13.328	1.00	45.66	A	C
ATOM	1453	CE1	TYR A 546	6.270	36.170	13.586	1.00	49.54	A	C
ATOM	1454	CZ	TYR A 546	5.194	36.185	14.476	1.00	51.88	A	C
ATOM	1455	OH	TYR A 546	4.527	37.365	14.649	1.00	56.67	A	O
ATOM	1456	CE2	TYR A 546	4.785	35.034	15.139	1.00	47.74	A	C
ATOM	1457	CD2	TYR A 546	5.465	33.828	14.854	1.00	46.25	A	C
ATOM	1458	C	TYR A 546	7.652	30.761	11.771	1.00	34.31	A	C
ATOM	1459	O	TYR A 546	8.817	31.027	11.364	1.00	33.34	A	O
ATOM	1460	N	TYR A 547	7.105	29.523	11.784	1.00	31.48	A	N
ATOM	1461	CA	TYR A 547	7.757	28.339	11.380	1.00	29.34	A	C
ATOM	1462	CB	TYR A 547	8.330	28.624	10.059	1.00	30.78	A	C
ATOM	1463	CG	TYR A 547	7.293	28.842	9.001	1.00	35.32	A	C
ATOM	1464	CD1	TYR A 547	5.960	28.995	9.290	1.00	34.90	A	C
ATOM	1465	CE1	TYR A 547	5.019	29.148	8.270	1.00	40.67	A	C
ATOM	1466	CZ	TYR A 547	5.487	29.181	6.930	1.00	45.72	A	C
ATOM	1467	OH	TYR A 547	4.710	29.304	5.815	1.00	46.53	A	O
ATOM	1468	CE2	TYR A 547	6.824	29.087	6.669	1.00	44.86	A	C
ATOM	1469	CD2	TYR A 547	7.687	28.895	7.674	1.00	41.03	A	C
ATOM	1470	C	TYR A 547	8.804	27.973	12.368	1.00	27.56	A	C
ATOM	1471	O	TYR A 547	9.794	27.305	12.101	1.00	24.39	A	O
ATOM	1472	N	LYS A 548	8.640	28.487	13.554	1.00	28.16	A	N
ATOM	1473	CA	LYS A 548	9.617	28.145	14.581	1.00	29.54	A	C
ATOM	1474	CB	LYS A 548	9.922	29.346	15.390	1.00	30.22	A	C
ATOM	1475	CG	LYS A 548	10.422	30.434	14.484	1.00	32.54	A	C
ATOM	1476	CD	LYS A 548	10.632	31.730	15.248	1.00	38.60	A	C
ATOM	1477	CE	LYS A 548	11.078	31.427	16.659	1.00	42.53	A	C
ATOM	1478	NZ	LYS A 548	11.916	32.498	17.292	1.00	47.49	A	N
ATOM	1479	C	LYS A 548	9.232	26.919	15.405	1.00	29.28	A	C
ATOM	1480	O	LYS A 548	8.099	26.812	15.810	1.00	30.47	A	O
ATOM	1481	N	PHE A 549	10.129	25.964	15.633	1.00	28.00	A	N
ATOM	1482	CA	PHE A 549	9.706	24.737	16.346	1.00	26.99	A	C
ATOM	1483	CB	PHE A 549	9.722	23.576	15.413	1.00	26.07	A	C
ATOM	1484	CG	PHE A 549	8.628	23.632	14.352	1.00	29.51	A	C
ATOM	1485	CD1	PHE A 549	8.789	24.351	13.162	1.00	26.22	A	C
ATOM	1486	CE1	PHE A 549	7.807	24.380	12.215	1.00	23.27	A	C
ATOM	1487	CZ	PHE A 549	6.675	23.718	12.403	1.00	26.76	A	C



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## Figure 2A - 25

ATOM	1488	CE2	PHE	A	549	6.444	23.016	13.606	1.00	27.87	A	C
ATOM	1489	CD2	PHE	A	549	7.377	22.973	14.563	1.00	28.75	A	C
ATOM	1490	C	PHE	A	549	10.615	24.426	17.433	1.00	26.57	A	C
ATOM	1491	O	PHE	A	549	11.757	24.134	17.201	1.00	28.34	A	O
ATOM	1492	N	SER	A	550	10.126	24.372	18.618	1.00	25.49	A	N
ATOM	1493	CA	SER	A	550	10.958	24.092	19.760	1.00	25.24	A	C
ATOM	1494	CB	SER	A	550	11.067	25.346	20.571	1.00	25.89	A	C
ATOM	1495	OG	SER	A	550	9.848	25.642	21.296	1.00	26.07	A	O
ATOM	1496	C	SER	A	550	10.356	23.038	20.687	1.00	24.63	A	C
ATOM	1497	O	SER	A	550	9.281	22.580	20.465	1.00	23.65	A	O
ATOM	1498	N	SER	A	551	11.070	22.646	21.725	1.00	24.63	A	N
ATOM	1499	CA	SER	A	551	10.444	21.770	22.720	1.00	25.71	A	C
ATOM	1500	CB	SER	A	551	11.388	21.446	23.819	1.00	25.46	A	C
ATOM	1501	OG	SER	A	551	12.134	20.464	23.316	1.00	25.45	A	O
ATOM	1502	C	SER	A	551	9.109	22.261	23.299	1.00	24.82	A	C
ATOM	1503	O	SER	A	551	8.120	21.486	23.488	1.00	24.21	A	O
ATOM	1504	N	LYS	A	552	9.073	23.541	23.526	1.00	23.98	A	N
ATOM	1505	CA	LYS	A	552	7.878	24.216	23.908	1.00	26.41	A	C
ATOM	1506	CB	LYS	A	552	8.252	25.653	24.395	1.00	27.66	A	C
ATOM	1507	CG	LYS	A	552	8.987	25.585	25.725	1.00	27.03	A	C
ATOM	1508	CD	LYS	A	552	9.079	26.861	26.249	1.00	31.86	A	C
ATOM	1509	CE	LYS	A	552	9.580	26.884	27.664	1.00	36.80	A	C
ATOM	1510	NZ	LYS	A	552	8.666	27.973	28.155	1.00	41.18	A	N
ATOM	1511	C	LYS	A	552	6.722	24.143	22.920	1.00	26.12	A	C
ATOM	1512	O	LYS	A	552	5.566	23.972	23.305	1.00	27.01	A	O
ATOM	1513	N	SER	A	553	6.995	24.220	21.646	1.00	26.17	A	N
ATOM	1514	CA	SER	A	553	5.946	23.867	20.728	1.00	27.28	A	C
ATOM	1515	CB	SER	A	553	6.349	23.957	19.252	1.00	28.38	A	C
ATOM	1516	OG	SER	A	553	7.222	24.995	19.005	1.00	31.12	A	O
ATOM	1517	C	SER	A	553	5.444	22.452	20.840	1.00	27.30	A	C
ATOM	1518	O	SER	A	553	4.277	22.243	20.597	1.00	29.22	A	O
ATOM	1519	N	ASP	A	554	6.294	21.479	21.071	1.00	25.56	A	N
ATOM	1520	CA	ASP	A	554	5.850	20.118	21.142	1.00	27.45	A	C
ATOM	1521	CB	ASP	A	554	7.054	19.077	21.411	1.00	29.02	A	C
ATOM	1522	CG	ASP	A	554	7.886	18.687	20.151	1.00	25.65	A	C
ATOM	1523	OD1	ASP	A	554	7.369	18.631	19.013	1.00	23.74	A	O
ATOM	1524	OD2	ASP	A	554	9.113	18.446	20.233	1.00	22.35	A	O
ATOM	1525	C	ASP	A	554	4.955	20.113	22.398	1.00	28.05	A	C
ATOM	1526	O	ASP	A	554	3.947	19.369	22.471	1.00	28.42	A	O
ATOM	1527	N	VAL	A	555	5.325	20.909	23.410	1.00	26.81	A	N
ATOM	1528	CA	VAL	A	555	4.470	20.990	24.580	1.00	25.45	A	C
ATOM	1529	CB	VAL	A	555	5.043	21.976	25.681	1.00	26.14	A	C
ATOM	1530	CG1	VAL	A	555	3.887	22.262	26.689	1.00	25.40	A	C
ATOM	1531	CG2	VAL	A	555	6.233	21.333	26.371	1.00	22.97	A	C
ATOM	1532	C	VAL	A	555	2.972	21.342	24.246	1.00	23.74	A	C
ATOM	1533	O	VAL	A	555	1.998	20.648	24.632	1.00	18.21	A	O
ATOM	1534	N	TRP	A	556	2.819	22.436	23.497	1.00	23.73	A	N
ATOM	1535	CA	TRP	A	556	1.494	22.698	22.933	1.00	23.81	A	C
ATOM	1536	CB	TRP	A	556	1.511	23.791	21.866	1.00	24.74	A	C
ATOM	1537	CG	TRP	A	556	0.103	24.212	21.311	1.00	25.59	A	C
ATOM	1538	CD1	TRP	A	556	-0.713	23.481	20.491	1.00	23.35	A	C
ATOM	1539	NE1	TRP	A	556	-1.868	24.165	20.292	1.00	19.70	A	N
ATOM	1540	CE2	TRP	A	556	-1.793	25.361	20.950	1.00	23.16	A	C
ATOM	1541	CD2	TRP	A	556	-0.585	25.429	21.567	1.00	23.47	A	C
ATOM	1542	CE3	TRP	A	556	-0.312	26.549	22.329	1.00	25.61	A	C
ATOM	1543	CZ3	TRP	A	556	-1.205	27.539	22.396	1.00	22.59	A	C
ATOM	1544	CH2	TRP	A	556	-2.369	27.470	21.774	1.00	22.11	A	C
ATOM	1545	CZ2	TRP	A	556	-2.694	26.404	21.011	1.00	26.21	A	C
ATOM	1546	C	TRP	A	556	0.885	21.389	22.314	1.00	21.81	A	C
ATOM	1547	O	TRP	A	556	-0.288	21.038	22.583	1.00	19.01	A	O
ATOM	1548	N	SER	A	557	1.655	20.644	21.541	1.00	19.68	A	N
ATOM	1549	CA	SER	A	557	1.029	19.524	20.907	1.00	21.19	A	C

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Figure 2A - 26

ATOM	1550	CB	SER A 557	1.997	18.855	19.950	1.00	22.36	A	C
ATOM	1551	OG	SER A 557	2.556	19.830	19.123	1.00	26.12	A	O
ATOM	1552	C	SER A 557	0.653	18.529	22.009	1.00	20.76	A	C
ATOM	1553	O	SER A 557	-0.328	17.839	21.972	1.00	18.77	A	O
ATOM	1554	N	PHE A 558	1.509	18.426	22.987	1.00	20.74	A	N
ATOM	1555	CA	PHE A 558	1.220	17.573	24.073	1.00	21.28	A	C
ATOM	1556	CB	PHE A 558	2.323	17.656	25.113	1.00	20.50	A	C
ATOM	1557	CG	PHE A 558	2.133	16.723	26.210	1.00	22.53	A	C
ATOM	1558	CD1	PHE A 558	2.303	15.358	25.985	1.00	23.02	A	C
ATOM	1559	CE1	PHE A 558	2.073	14.439	27.036	1.00	25.64	A	C
ATOM	1560	CZ	PHE A 558	1.678	14.869	28.353	1.00	24.82	A	C
ATOM	1561	CE2	PHE A 558	1.508	16.237	28.579	1.00	24.14	A	C
ATOM	1562	CD2	PHE A 558	1.712	17.182	27.504	1.00	22.51	A	C
ATOM	1563	C	PHE A 558	-0.163	17.940	24.597	1.00	21.22	A	C
ATOM	1564	O	PHE A 558	-1.005	17.051	24.839	1.00	21.95	A	O
ATOM	1565	N	GLY A 559	-0.434	19.230	24.685	1.00	18.90	A	N
ATOM	1566	CA	GLY A 559	-1.694	19.646	25.170	1.00	18.86	A	C
ATOM	1567	C	GLY A 559	-2.852	19.011	24.419	1.00	21.32	A	C
ATOM	1568	O	GLY A 559	-3.752	18.434	25.099	1.00	19.02	A	O
ATOM	1569	N	VAL A 560	-2.851	19.149	23.050	1.00	19.78	A	N
ATOM	1570	CA	VAL A 560	-3.900	18.620	22.259	1.00	18.84	A	C
ATOM	1571	CB	VAL A 560	-3.540	18.834	20.737	1.00	20.05	A	C
ATOM	1572	CG1	VAL A 560	-4.495	18.117	19.837	1.00	18.50	A	C
ATOM	1573	CG2	VAL A 560	-3.360	20.241	20.425	1.00	19.01	A	C
ATOM	1574	C	VAL A 560	-3.972	17.129	22.460	1.00	18.51	A	C
ATOM	1575	O	VAL A 560	-4.984	16.556	22.434	1.00	17.10	A	O
ATOM	1576	N	LEU A 561	-2.863	16.456	22.610	1.00	20.01	A	N
ATOM	1577	CA	LEU A 561	-2.896	15.012	22.741	1.00	22.20	A	C
ATOM	1578	CB	LEU A 561	-1.473	14.433	22.612	1.00	23.11	A	C
ATOM	1579	CG	LEU A 561	-0.988	12.974	22.834	1.00	26.47	A	C
ATOM	1580	CD1	LEU A 561	0.437	12.879	22.306	1.00	24.08	A	C
ATOM	1581	CD2	LEU A 561	-1.051	12.603	24.261	1.00	27.64	A	C
ATOM	1582	C	LEU A 561	-3.512	14.688	24.141	1.00	23.25	A	C
ATOM	1583	O	LEU A 561	-4.318	13.743	24.267	1.00	24.63	A	O
ATOM	1584	N	MET A 562	-3.188	15.429	25.164	1.00	21.48	A	N
ATOM	1585	CA	MET A 562	-3.901	15.126	26.401	1.00	24.97	A	C
ATOM	1586	CB	MET A 562	-3.555	16.084	27.578	1.00	24.51	A	C
ATOM	1587	CG	MET A 562	-2.137	15.952	28.059	1.00	27.41	A	C
ATOM	1588	SD	MET A 562	-1.735	16.867	29.547	1.00	29.10	A	S
ATOM	1589	CE	MET A 562	-2.937	16.128	30.342	1.00	31.73	A	C
ATOM	1590	C	MET A 562	-5.443	15.126	26.166	1.00	24.47	A	C
ATOM	1591	O	MET A 562	-6.178	14.141	26.519	1.00	22.02	A	O
ATOM	1592	N	TRP A 563	-5.886	16.204	25.544	1.00	23.91	A	N
ATOM	1593	CA	TRP A 563	-7.298	16.337	25.279	1.00	25.50	A	C
ATOM	1594	CB	TRP A 563	-7.576	17.730	24.700	1.00	25.25	A	C
ATOM	1595	CG	TRP A 563	-9.080	17.946	24.266	1.00	26.09	A	C
ATOM	1596	CD1	TRP A 563	-9.966	18.794	24.825	1.00	23.94	A	C
ATOM	1597	NE1	TRP A 563	-11.167	18.757	24.159	1.00	21.95	A	N
ATOM	1598	CE2	TRP A 563	-11.088	17.911	23.107	1.00	26.57	A	C
ATOM	1599	CD2	TRP A 563	-9.752	17.398	23.097	1.00	27.47	A	C
ATOM	1600	CE3	TRP A 563	-9.387	16.499	22.092	1.00	20.91	A	C
ATOM	1601	CZ3	TRP A 563	-10.346	16.131	21.161	1.00	22.21	A	C
ATOM	1602	CH2	TRP A 563	-11.680	16.636	21.212	1.00	23.35	A	C
ATOM	1603	CZ2	TRP A 563	-12.056	17.550	22.157	1.00	25.73	A	C
ATOM	1604	C	TRP A 563	-7.908	15.187	24.421	1.00	25.06	A	C
ATOM	1605	O	TRP A 563	-9.005	14.763	24.649	1.00	24.03	A	O
ATOM	1606	N	GLU A 564	-7.182	14.699	23.432	1.00	24.60	A	N
ATOM	1607	CA	GLU A 564	-7.672	13.559	22.641	1.00	23.98	A	C
ATOM	1608	CB	GLU A 564	-6.750	13.225	21.449	1.00	22.98	A	C
ATOM	1609	CG	GLU A 564	-6.300	14.328	20.553	1.00	22.89	A	C
ATOM	1610	CD	GLU A 564	-5.257	13.839	19.508	1.00	28.53	A	C
ATOM	1611	OE1	GLU A 564	-4.017	14.094	19.786	1.00	26.20	A	O

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ATOM	1612	OE2	GLU	A	564	-5.662	13.222	18.397	1.00	26.34	A	O
ATOM	1613	C	GLU	A	564	-7.734	12.314	23.572	1.00	23.28	A	C
ATOM	1614	O	GLU	A	564	-8.683	11.518	23.491	1.00	21.86	A	O
ATOM	1615	N	ALA	A	565	-6.678	12.119	24.361	1.00	21.47	A	N
ATOM	1616	CA	ALA	A	565	-6.684	11.012	25.262	1.00	23.08	A	C
ATOM	1617	CB	ALA	A	565	-5.364	10.798	25.959	1.00	22.41	A	C
ATOM	1618	C	ALA	A	565	-7.838	11.001	26.252	1.00	23.38	A	C
ATOM	1619	O	ALA	A	565	-8.404	10.011	26.442	1.00	23.38	A	O
ATOM	1620	N	PHE	A	566	-8.207	12.089	26.863	1.00	24.94	A	N
ATOM	1621	CA	PHE	A	566	-9.426	12.053	27.702	1.00	26.55	A	C
ATOM	1622	CB	PHE	A	566	-9.360	13.128	28.788	1.00	25.87	A	C
ATOM	1623	CG	PHE	A	566	-8.212	12.962	29.687	1.00	27.26	A	C
ATOM	1624	CD1	PHE	A	566	-8.363	12.327	30.914	1.00	27.28	A	C
ATOM	1625	CE1	PHE	A	566	-7.324	12.160	31.754	1.00	24.21	A	C
ATOM	1626	CZ	PHE	A	566	-6.137	12.651	31.415	1.00	27.54	A	C
ATOM	1627	CE2	PHE	A	566	-5.928	13.256	30.199	1.00	28.95	A	C
ATOM	1628	CD2	PHE	A	566	-6.976	13.434	29.348	1.00	27.06	A	C
ATOM	1629	C	PHE	A	566	-10.776	12.140	26.940	1.00	26.89	A	C
ATOM	1630	O	PHE	A	566	-11.829	12.121	27.500	1.00	26.15	A	O
ATOM	1631	N	SER	A	567	-10.737	12.294	25.631	1.00	27.98	A	N
ATOM	1632	CA	SER	A	567	-11.921	12.359	24.825	1.00	27.51	A	C
ATOM	1633	CB	SER	A	567	-11.712	13.415	23.751	1.00	25.84	A	C
ATOM	1634	OG	SER	A	567	-11.648	14.711	24.369	1.00	23.87	A	O
ATOM	1635	C	SER	A	567	-12.009	10.986	24.197	1.00	30.22	A	C
ATOM	1636	O	SER	A	567	-12.709	10.780	23.181	1.00	32.61	A	O
ATOM	1637	N	TYR	A	568	-11.235	10.054	24.713	1.00	30.36	A	N
ATOM	1638	CA	TYR	A	568	-11.176	8.751	24.102	1.00	31.01	A	C
ATOM	1639	CB	TYR	A	568	-12.364	7.893	24.547	1.00	32.52	A	C
ATOM	1640	CG	TYR	A	568	-12.387	7.733	26.082	1.00	33.00	A	C
ATOM	1641	CD1	TYR	A	568	-11.910	6.599	26.641	1.00	34.43	A	C
ATOM	1642	CE1	TYR	A	568	-11.950	6.388	28.059	1.00	38.44	A	C
ATOM	1643	CZ	TYR	A	568	-12.479	7.334	28.888	1.00	39.46	A	C
ATOM	1644	OH	TYR	A	568	-12.379	6.988	30.215	1.00	43.02	A	O
ATOM	1645	CE2	TYR	A	568	-13.043	8.539	28.353	1.00	35.43	A	C
ATOM	1646	CD2	TYR	A	568	-12.943	8.740	26.953	1.00	33.94	A	C
ATOM	1647	C	TYR	A	568	-10.964	8.766	22.566	1.00	30.48	A	C
ATOM	1648	O	TYR	A	568	-11.673	8.158	21.841	1.00	28.72	A	O
ATOM	1649	N	GLY	A	569	-9.921	9.450	22.135	1.00	29.96	A	N
ATOM	1650	CA	GLY	A	569	-9.423	9.334	20.819	1.00	30.15	A	C
ATOM	1651	C	GLY	A	569	-10.232	10.094	19.823	1.00	30.83	A	C
ATOM	1652	O	GLY	A	569	-10.153	9.808	18.679	1.00	30.57	A	O
ATOM	1653	N	GLN	A	570	-11.061	11.009	20.243	1.00	31.42	A	N
ATOM	1654	CA	GLN	A	570	-11.717	11.824	19.247	1.00	33.08	A	C
ATOM	1655	CB	GLN	A	570	-12.965	12.502	19.784	1.00	33.62	A	C
ATOM	1656	CG	GLN	A	570	-14.195	11.763	19.236	1.00	39.53	A	C
ATOM	1657	CD	GLN	A	570	-15.352	11.644	20.233	1.00	44.52	A	C
ATOM	1658	OE1	GLN	A	570	-16.114	10.614	20.155	1.00	49.45	A	O
ATOM	1659	NE2	GLN	A	570	-15.471	12.641	21.212	1.00	40.15	A	N
ATOM	1660	C	GLN	A	570	-10.776	12.864	18.652	1.00	32.61	A	C
ATOM	1661	O	GLN	A	570	-9.946	13.350	19.358	1.00	31.93	A	O
ATOM	1662	N	LYS	A	571	-10.904	13.165	17.370	1.00	31.37	A	N
ATOM	1663	CA	LYS	A	571	-10.191	14.292	16.815	1.00	31.89	A	C
ATOM	1664	CB	LYS	A	571	-10.512	14.350	15.321	1.00	33.29	A	C
ATOM	1665	CG	LYS	A	571	-10.536	12.968	14.722	1.00	38.44	A	C
ATOM	1666	CD	LYS	A	571	-10.586	12.951	13.102	1.00	43.18	A	C
ATOM	1667	CE	LYS	A	571	-9.175	12.540	12.489	1.00	39.78	A	C
ATOM	1668	NZ	LYS	A	571	-8.905	11.081	12.463	1.00	34.52	A	N
ATOM	1669	C	LYS	A	571	-10.443	15.643	17.466	1.00	30.25	A	C
ATOM	1670	O	LYS	A	571	-11.525	15.950	17.989	1.00	31.75	A	O
ATOM	1671	N	PRO	A	572	-9.440	16.483	17.522	1.00	28.24	A	N
ATOM	1672	CA	PRO	A	572	-9.622	17.835	18.075	1.00	27.80	A	C
ATOM	1673	CB	PRO	A	572	-8.186	18.275	18.389	1.00	28.47	A	C

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## Figure 2A - 28

ATOM	1674	CG	PRO	A	572	-7.364	17.531	17.343	1.00	28.01	A	C
ATOM	1675	CD	PRO	A	572	-8.046	16.200	17.173	1.00	27.81	A	C
ATOM	1676	C	PRO	A	572	-10.224	18.768	17.033	1.00	27.21	A	C
ATOM	1677	O	PRO	A	572	-10.172	18.443	15.857	1.00	25.01	A	O
ATOM	1678	N	TYR	A	573	-10.758	19.913	17.477	1.00	27.25	A	N
ATOM	1679	CA	TYR	A	573	-11.345	20.881	16.598	1.00	27.73	A	C
ATOM	1680	CB	TYR	A	573	-10.249	21.778	16.059	1.00	28.98	A	C
ATOM	1681	CG	TYR	A	573	-9.247	22.275	17.070	1.00	24.98	A	C
ATOM	1682	CD1	TYR	A	573	-9.485	23.356	17.820	1.00	24.81	A	C
ATOM	1683	CE1	TYR	A	573	-8.592	23.785	18.771	1.00	26.12	A	C
ATOM	1684	CZ	TYR	A	573	-7.420	23.140	18.881	1.00	25.70	A	C
ATOM	1685	OH	TYR	A	573	-6.422	23.552	19.753	1.00	22.76	A	O
ATOM	1686	CE2	TYR	A	573	-7.218	22.057	18.117	1.00	24.24	A	C
ATOM	1687	CD2	TYR	A	573	-8.065	21.683	17.194	1.00	22.63	A	C
ATOM	1688	C	TYR	A	573	-12.195	20.268	15.458	1.00	29.43	A	C
ATOM	1689	O	TYR	A	573	-12.083	20.609	14.235	1.00	27.00	A	O
ATOM	1690	N	ARG	A	574	-13.031	19.313	15.829	1.00	30.68	A	N
ATOM	1691	CA	ARG	A	574	-13.831	18.718	14.791	1.00	33.07	A	C
ATOM	1692	CB	ARG	A	574	-14.705	17.567	15.282	1.00	35.68	A	C
ATOM	1693	CG	ARG	A	574	-15.958	18.017	16.134	1.00	40.14	A	C
ATOM	1694	CD	ARG	A	574	-16.786	16.740	16.755	1.00	43.73	A	C
ATOM	1695	NE	ARG	A	574	-17.823	17.266	17.656	1.00	45.09	A	N
ATOM	1696	CZ	ARG	A	574	-18.264	16.756	18.794	1.00	42.87	A	C
ATOM	1697	NH1	ARG	A	574	-17.849	15.597	19.190	1.00	39.22	A	N
ATOM	1698	NH2	ARG	A	574	-19.192	17.421	19.530	1.00	42.77	A	N
ATOM	1699	C	ARG	A	574	-14.703	19.755	14.088	1.00	31.83	A	C
ATOM	1700	O	ARG	A	574	-15.157	20.753	14.655	1.00	28.13	A	O
ATOM	1701	N	GLY	A	575	-14.888	19.455	12.821	1.00	31.14	A	N
ATOM	1702	CA	GLY	A	575	-15.682	20.255	11.979	1.00	33.01	A	C
ATOM	1703	C	GLY	A	575	-14.964	21.498	11.577	1.00	35.34	A	C
ATOM	1704	O	GLY	A	575	-15.578	22.304	10.917	1.00	38.05	A	O
ATOM	1705	N	MET	A	576	-13.696	21.677	11.909	1.00	34.43	A	N
ATOM	1706	CA	MET	A	576	-13.028	22.937	11.628	1.00	33.96	A	C
ATOM	1707	CB	MET	A	576	-12.601	23.577	12.918	1.00	32.20	A	C
ATOM	1708	CG	MET	A	576	-13.739	23.950	13.825	1.00	28.36	A	C
ATOM	1709	SD	MET	A	576	-13.162	24.579	15.564	1.00	27.21	A	S
ATOM	1710	CE	MET	A	576	-12.535	26.252	15.152	1.00	22.40	A	C
ATOM	1711	C	MET	A	576	-11.796	22.820	10.663	1.00	36.13	A	C
ATOM	1712	O	MET	A	576	-11.091	21.730	10.569	1.00	35.51	A	O
ATOM	1713	N	LYS	A	577	-11.569	23.918	9.932	1.00	35.77	A	N
ATOM	1714	CA	LYS	A	577	-10.366	24.049	9.070	1.00	36.01	A	C
ATOM	1715	CB	LYS	A	577	-10.585	25.093	7.942	1.00	36.47	A	C
ATOM	1716	CG	LYS	A	577	-11.470	24.644	6.698	1.00	40.93	A	C
ATOM	1717	CD	LYS	A	577	-12.054	25.896	5.970	1.00	46.21	A	C
ATOM	1718	CE	LYS	A	577	-13.650	26.009	6.030	1.00	51.15	A	C
ATOM	1719	NZ	LYS	A	577	-14.354	27.408	5.807	1.00	49.80	A	N
ATOM	1720	C	LYS	A	577	-9.215	24.560	9.959	1.00	34.70	A	C
ATOM	1721	O	LYS	A	577	-9.470	25.172	11.013	1.00	32.49	A	O
ATOM	1722	N	GLY	A	578	-7.968	24.337	9.487	1.00	33.54	A	N
ATOM	1723	CA	GLY	A	578	-6.764	24.832	10.125	1.00	31.58	A	C
ATOM	1724	C	GLY	A	578	-6.894	26.316	10.324	1.00	31.35	A	C
ATOM	1725	O	GLY	A	578	-6.501	26.944	11.373	1.00	29.55	A	O
ATOM	1726	N	SER	A	579	-7.464	26.960	9.329	1.00	30.69	A	N
ATOM	1727	CA	SER	A	579	-7.435	28.393	9.488	1.00	30.90	A	C
ATOM	1728	CB	SER	A	579	-7.665	28.960	8.131	1.00	32.52	A	C
ATOM	1729	OG	SER	A	579	-8.955	28.489	7.679	1.00	35.04	A	O
ATOM	1730	C	SER	A	579	-8.504	28.837	10.514	1.00	29.24	A	C
ATOM	1731	O	SER	A	579	-8.477	29.896	11.116	1.00	28.41	A	O
ATOM	1732	N	GLU	A	580	-9.505	28.045	10.663	1.00	28.29	A	N
ATOM	1733	CA	GLU	A	580	-10.540	28.411	11.631	1.00	30.12	A	C
ATOM	1734	CB	GLU	A	580	-11.847	27.604	11.361	1.00	30.31	A	C
ATOM	1735	CG	GLU	A	580	-12.571	28.101	10.111	1.00	34.57	A	C

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## Figure 2A - 29

ATOM	1736	CD	GLU	A	580	-13.483	27.071	9.463	1.00	37.43	A	C
ATOM	1737	OE1	GLU	A	580	-13.144	25.871	9.359	1.00	40.16	A	O
ATOM	1738	OE2	GLU	A	580	-14.583	27.462	9.082	1.00	37.91	A	O
ATOM	1739	C	GLU	A	580	-9.997	28.186	13.126	1.00	28.02	A	C
ATOM	1740	O	GLU	A	580	-10.375	28.878	14.043	1.00	28.31	A	O
ATOM	1741	N	VAL	A	581	-9.156	27.210	13.290	1.00	25.45	A	N
ATOM	1742	CA	VAL	A	581	-8.452	26.992	14.522	1.00	26.26	A	C
ATOM	1743	CB	VAL	A	581	-7.786	25.551	14.504	1.00	26.43	A	C
ATOM	1744	CG1	VAL	A	581	-6.939	25.309	15.716	1.00	20.87	A	C
ATOM	1745	CG2	VAL	A	581	-8.907	24.468	14.184	1.00	20.69	A	C
ATOM	1746	C	VAL	A	581	-7.480	28.123	14.827	1.00	27.40	A	C
ATOM	1747	O	VAL	A	581	-7.515	28.773	15.998	1.00	26.42	A	O
ATOM	1748	N	THR	A	582	-6.620	28.421	13.827	1.00	26.18	A	N
ATOM	1749	CA	THR	A	582	-5.753	29.602	13.984	1.00	26.96	A	C
ATOM	1750	CB	THR	A	582	-4.951	29.891	12.766	1.00	26.86	A	C
ATOM	1751	OG1	THR	A	582	-3.833	28.979	12.719	1.00	29.18	A	O
ATOM	1752	CG2	THR	A	582	-4.226	31.106	12.934	1.00	26.99	A	C
ATOM	1753	C	THR	A	582	-6.572	30.833	14.460	1.00	28.33	A	C
ATOM	1754	O	THR	A	582	-6.278	31.447	15.541	1.00	28.82	A	O
ATOM	1755	N	ALA	A	583	-7.667	31.107	13.768	1.00	26.82	A	N
ATOM	1756	CA	ALA	A	583	-8.476	32.187	14.214	1.00	28.20	A	C
ATOM	1757	CB	ALA	A	583	-9.595	32.558	13.219	1.00	28.65	A	C
ATOM	1758	C	ALA	A	583	-9.066	31.972	15.585	1.00	28.67	A	C
ATOM	1759	O	ALA	A	583	-9.120	32.890	16.341	1.00	27.61	A	O
ATOM	1760	N	MET	A	584	-9.556	30.780	15.889	1.00	29.89	A	N
ATOM	1761	CA	MET	A	584	-10.073	30.532	17.214	1.00	30.91	A	C
ATOM	1762	CB	MET	A	584	-10.603	29.095	17.214	1.00	32.45	A	C
ATOM	1763	CG	MET	A	584	-11.009	28.596	18.636	1.00	32.51	A	C
ATOM	1764	SD	MET	A	584	-11.515	26.980	18.523	1.00	31.14	A	S
ATOM	1765	CE	MET	A	584	-11.741	26.664	20.525	1.00	23.52	A	C
ATOM	1766	C	MET	A	584	-9.034	30.780	18.340	1.00	31.16	A	C
ATOM	1767	O	MET	A	584	-9.294	31.506	19.317	1.00	31.66	A	O
ATOM	1768	N	LEU	A	585	-7.819	30.250	18.176	1.00	31.44	A	N
ATOM	1769	CA	LEU	A	585	-6.776	30.359	19.207	1.00	32.04	A	C
ATOM	1770	CB	LEU	A	585	-5.578	29.423	18.899	1.00	31.54	A	C
ATOM	1771	CG	LEU	A	585	-5.971	27.920	18.944	1.00	30.70	A	C
ATOM	1772	CD1	LEU	A	585	-4.832	27.095	18.453	1.00	31.63	A	C
ATOM	1773	CD2	LEU	A	585	-6.375	27.474	20.358	1.00	21.24	A	C
ATOM	1774	C	LEU	A	585	-6.363	31.789	19.461	1.00	32.97	A	C
ATOM	1775	O	LEU	A	585	-6.130	32.201	20.588	1.00	32.93	A	O
ATOM	1776	N	GLU	A	586	-6.248	32.547	18.395	1.00	34.88	A	N
ATOM	1777	CA	GLU	A	586	-5.873	33.979	18.458	1.00	36.45	A	C
ATOM	1778	CB	GLU	A	586	-5.708	34.598	17.070	1.00	38.54	A	C
ATOM	1779	CG	GLU	A	586	-5.720	36.116	17.022	1.00	43.74	A	C
ATOM	1780	CD	GLU	A	586	-5.161	36.696	15.666	1.00	48.50	A	C
ATOM	1781	OE1	GLU	A	586	-4.343	35.961	14.973	1.00	49.85	A	O
ATOM	1782	OE2	GLU	A	586	-5.505	37.895	15.329	1.00	45.61	A	O
ATOM	1783	C	GLU	A	586	-6.838	34.826	19.257	1.00	35.24	A	C
ATOM	1784	O	GLU	A	586	-6.365	35.792	19.835	1.00	35.53	A	O
ATOM	1785	N	LYS	A	587	-8.135	34.479	19.313	1.00	32.79	A	N
ATOM	1786	CA	LYS	A	587	-9.100	35.231	20.108	1.00	31.67	A	C
ATOM	1787	CB	LYS	A	587	-10.482	34.966	19.670	1.00	31.64	A	C
ATOM	1788	CG	LYS	A	587	-10.985	35.461	18.345	1.00	38.39	A	C
ATOM	1789	CD	LYS	A	587	-12.404	34.766	18.113	1.00	43.33	A	C
ATOM	1790	CE	LYS	A	587	-12.896	34.978	16.682	1.00	47.08	A	C
ATOM	1791	NZ	LYS	A	587	-14.378	34.722	16.609	1.00	50.34	A	N
ATOM	1792	C	LYS	A	587	-9.091	34.724	21.621	1.00	32.13	A	C
ATOM	1793	O	LYS	A	587	-9.999	35.113	22.434	1.00	28.80	A	O
ATOM	1794	N	GLY	A	588	-8.153	33.809	21.950	1.00	31.47	A	N
ATOM	1795	CA	GLY	A	588	-8.017	33.287	23.297	1.00	31.14	A	C
ATOM	1796	C	GLY	A	588	-8.912	32.079	23.467	1.00	31.04	A	C
ATOM	1797	O	GLY	A	588	-9.064	31.552	24.549	1.00	29.66	A	O

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ATOM	1798	N	GLU	A	589	-9.524	31.587	22.389	1.00	30.71	A	N
ATOM	1799	CA	GLU	A	589	-10.496	30.493	22.708	1.00	29.70	A	C
ATOM	1800	CB	GLU	A	589	-11.687	30.523	21.755	1.00	30.31	A	C
ATOM	1801	CG	GLU	A	589	-12.660	31.648	22.045	1.00	29.93	A	C
ATOM	1802	CD	GLU	A	589	-13.520	31.997	20.839	1.00	35.97	A	C
ATOM	1803	OE1	GLU	A	589	-13.608	31.160	19.834	1.00	31.80	A	O
ATOM	1804	OE2	GLU	A	589	-14.151	33.121	20.936	1.00	39.74	A	O
ATOM	1805	C	GLU	A	589	-9.807	29.131	22.641	1.00	28.26	A	C
ATOM	1806	O	GLU	A	589	-8.795	28.986	21.926	1.00	24.72	A	O
ATOM	1807	N	ARG	A	590	-10.339	28.202	23.442	1.00	27.05	A	N
ATOM	1808	CA	ARG	A	590	-9.809	26.871	23.606	1.00	27.66	A	C
ATOM	1809	CB	ARG	A	590	-9.066	26.734	24.934	1.00	27.15	A	C
ATOM	1810	CG	ARG	A	590	-7.945	27.634	25.067	1.00	26.56	A	C
ATOM	1811	CD	ARG	A	590	-6.967	27.554	23.938	1.00	27.57	A	C
ATOM	1812	NE	ARG	A	590	-5.736	28.280	24.184	1.00	27.29	A	N
ATOM	1813	CZ	ARG	A	590	-5.462	29.416	23.579	1.00	27.02	A	C
ATOM	1814	NH1	ARG	A	590	-6.347	29.943	22.714	1.00	25.26	A	N
ATOM	1815	NH2	ARG	A	590	-4.322	30.021	23.845	1.00	24.36	A	N
ATOM	1816	C	ARG	A	590	-10.925	25.835	23.557	1.00	27.94	A	C
ATOM	1817	O	ARG	A	590	-12.066	26.098	23.923	1.00	25.01	A	O
ATOM	1818	N	MET	A	591	-10.491	24.631	23.250	1.00	29.37	A	N
ATOM	1819	CA	MET	A	591	-11.298	23.457	23.109	1.00	33.47	A	C
ATOM	1820	CB	MET	A	591	-10.456	22.231	22.743	1.00	33.50	A	C
ATOM	1821	CG	MET	A	591	-10.429	21.950	21.323	1.00	31.94	A	C
ATOM	1822	SD	MET	A	591	-9.648	20.412	20.952	1.00	30.35	A	S
ATOM	1823	CE	MET	A	591	-7.997	20.691	21.291	1.00	27.47	A	C
ATOM	1824	C	MET	A	591	-12.267	23.006	24.167	1.00	36.18	A	C
ATOM	1825	O	MET	A	591	-13.291	22.339	23.820	1.00	39.83	A	O
ATOM	1826	N	GLY	A	592	-12.104	23.229	25.440	1.00	36.53	A	N
ATOM	1827	CA	GLY	A	592	-13.345	22.721	26.133	1.00	34.29	A	C
ATOM	1828	C	GLY	A	592	-13.051	21.386	26.812	1.00	33.11	A	C
ATOM	1829	O	GLY	A	592	-12.594	20.489	26.128	1.00	31.88	A	O
ATOM	1830	N	CYS	A	593	-13.192	21.302	28.146	1.00	32.16	A	N
ATOM	1831	CA	CYS	A	593	-12.958	20.103	28.969	1.00	32.11	A	C
ATOM	1832	CB	CYS	A	593	-13.243	20.403	30.450	1.00	32.20	A	C
ATOM	1833	SG	CYS	A	593	-12.844	19.086	31.584	1.00	31.73	A	S
ATOM	1834	C	CYS	A	593	-13.772	18.917	28.532	1.00	33.50	A	C
ATOM	1835	O	CYS	A	593	-15.026	18.928	28.302	1.00	33.65	A	O
ATOM	1836	N	PRO	A	594	-13.034	17.883	28.289	1.00	33.64	A	N
ATOM	1837	CA	PRO	A	594	-13.641	16.637	27.850	1.00	35.59	A	C
ATOM	1838	CB	PRO	A	594	-12.452	15.717	27.579	1.00	34.93	A	C
ATOM	1839	CG	PRO	A	594	-11.243	16.676	27.420	1.00	32.50	A	C
ATOM	1840	CD	PRO	A	594	-11.575	17.859	28.350	1.00	33.62	A	C
ATOM	1841	C	PRO	A	594	-14.598	16.077	28.914	1.00	36.59	A	C
ATOM	1842	O	PRO	A	594	-14.305	16.055	30.131	1.00	37.87	A	O
ATOM	1843	N	ALA	A	595	-15.710	15.564	28.449	1.00	36.72	A	N
ATOM	1844	CA	ALA	A	595	-16.714	15.069	29.409	1.00	39.43	A	C
ATOM	1845	CB	ALA	A	595	-17.939	14.392	28.684	1.00	40.34	A	C
ATOM	1846	C	ALA	A	595	-16.137	14.147	30.447	1.00	38.53	A	C
ATOM	1847	O	ALA	A	595	-15.557	13.102	30.098	1.00	38.08	A	O
ATOM	1848	N	GLY	A	596	-16.282	14.515	31.718	1.00	38.23	A	N
ATOM	1849	CA	GLY	A	596	-15.753	13.619	32.750	1.00	38.43	A	C
ATOM	1850	C	GLY	A	596	-14.210	13.707	32.915	1.00	38.54	A	C
ATOM	1851	O	GLY	A	596	-13.644	12.894	33.624	1.00	38.79	A	O
ATOM	1852	N	CYS	A	597	-13.546	14.712	32.319	1.00	36.97	A	N
ATOM	1853	CA	CYS	A	597	-12.115	14.884	32.507	1.00	36.30	A	C
ATOM	1854	CB	CYS	A	597	-11.583	15.853	31.393	1.00	36.37	A	C
ATOM	1855	SG	CYS	A	597	-9.796	15.846	31.381	1.00	29.42	A	S
ATOM	1856	C	CYS	A	597	-11.806	15.528	33.833	1.00	36.39	A	C
ATOM	1857	O	CYS	A	597	-12.473	16.440	34.148	1.00	36.19	A	O
ATOM	1858	N	PRO	A	598	-10.812	15.106	34.613	1.00	37.08	A	N
ATOM	1859	CA	PRO	A	598	-10.516	15.764	35.877	1.00	36.64	A	C

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ATOM	1860	CB	PRO	A	598	-9.387	14.932	36.452	1.00	36.23	A	C
ATOM	1861	CG	PRO	A	598	-9.498	13.706	35.782	1.00	37.84	A	C
ATOM	1862	CD	PRO	A	598	-9.829	14.036	34.363	1.00	37.74	A	C
ATOM	1863	C	PRO	A	598	-9.942	17.112	35.620	1.00	37.19	A	C
ATOM	1864	O	PRO	A	598	-9.176	17.399	34.694	1.00	38.27	A	O
ATOM	1865	N	ARG	A	599	-10.309	17.980	36.487	1.00	36.36	A	N
ATOM	1866	CA	ARG	A	599	-10.015	19.333	36.332	1.00	36.29	A	C
ATOM	1867	CB	ARG	A	599	-10.657	20.080	37.504	1.00	37.29	A	C
ATOM	1868	CG	ARG	A	599	-12.050	20.478	37.110	1.00	38.87	A	C
ATOM	1869	CD	ARG	A	599	-12.054	21.623	36.032	1.00	42.95	A	C
ATOM	1870	NE	ARG	A	599	-13.097	21.372	35.063	1.00	43.10	A	N
ATOM	1871	CZ	ARG	A	599	-13.570	22.261	34.287	1.00	45.31	A	C
ATOM	1872	NH1	ARG	A	599	-13.078	23.506	34.291	1.00	43.69	A	N
ATOM	1873	NH2	ARG	A	599	-14.546	21.893	33.482	1.00	48.71	A	N
ATOM	1874	C	ARG	A	599	-8.572	19.612	36.293	1.00	34.58	A	C
ATOM	1875	O	ARG	A	599	-8.151	20.461	35.562	1.00	33.42	A	O
ATOM	1876	N	GLU	A	600	-7.807	18.908	37.085	1.00	33.50	A	N
ATOM	1877	CA	GLU	A	600	-6.463	19.273	37.144	1.00	33.99	A	C
ATOM	1878	CB	GLU	A	600	-5.781	18.548	38.314	1.00	36.82	A	C
ATOM	1879	CG	AGLU	A	600	-6.550	17.348	38.886	0.70	39.62	A	C
ATOM	1880	CG	BGLU	A	600	-4.272	18.815	38.401	0.30	36.25	A	C
ATOM	1881	CD	AGLU	A	600	-7.740	17.675	39.787	0.70	43.44	A	C
ATOM	1882	CD	BGLU	A	600	-3.909	20.293	38.299	0.30	36.70	A	C
ATOM	1883	OE1	AGLU	A	600	-7.572	18.077	40.988	0.70	44.65	A	O
ATOM	1884	OE1	BGLU	A	600	-4.720	21.178	38.680	0.30	37.17	A	O
ATOM	1885	OE2	AGLU	A	600	-8.876	17.514	39.315	0.70	44.68	A	O
ATOM	1886	OE2	BGLU	A	600	-2.811	20.583	37.811	0.30	37.05	A	O
ATOM	1887	C	GLU	A	600	-5.788	19.021	35.810	1.00	32.54	A	C
ATOM	1888	O	GLU	A	600	-4.938	19.788	35.363	1.00	31.26	A	O
ATOM	1889	N	MET	A	601	-6.201	17.952	35.159	1.00	31.54	A	N
ATOM	1890	CA	MET	A	601	-5.752	17.631	33.810	1.00	30.69	A	C
ATOM	1891	CB	MET	A	601	-6.146	16.241	33.393	1.00	31.64	A	C
ATOM	1892	CG	MET	A	601	-5.534	15.167	34.468	1.00	35.27	A	C
ATOM	1893	SD	MET	A	601	-3.844	14.787	34.349	1.00	34.50	A	S
ATOM	1894	CE	MET	A	601	-2.948	15.972	35.306	1.00	37.46	A	C
ATOM	1895	C	MET	A	601	-6.132	18.670	32.813	1.00	29.38	A	C
ATOM	1896	O	MET	A	601	-5.256	19.196	32.227	1.00	28.57	A	O
ATOM	1897	N	TYR	A	602	-7.386	19.075	32.769	1.00	28.84	A	N
ATOM	1898	CA	TYR	A	602	-7.860	20.055	31.846	1.00	29.84	A	C
ATOM	1899	CB	TYR	A	602	-9.395	20.295	31.942	1.00	29.22	A	C
ATOM	1900	CG	TYR	A	602	-9.882	21.376	31.014	1.00	28.77	A	C
ATOM	1901	CD1	TYR	A	602	-9.721	21.153	29.615	1.00	26.76	A	C
ATOM	1902	CE1	TYR	A	602	-10.085	22.067	28.664	1.00	29.33	A	C
ATOM	1903	CZ	TYR	A	602	-10.699	23.324	29.035	1.00	35.97	A	C
ATOM	1904	OH	TYR	A	602	-11.050	24.147	27.869	1.00	34.22	A	O
ATOM	1905	CE2	TYR	A	602	-10.920	23.610	30.506	1.00	30.35	A	C
ATOM	1906	CD2	TYR	A	602	-10.484	22.621	31.478	1.00	27.46	A	C
ATOM	1907	C	TYR	A	602	-7.036	21.362	32.066	1.00	29.41	A	C
ATOM	1908	O	TYR	A	602	-6.589	21.989	31.089	1.00	28.91	A	O
ATOM	1909	N	ASP	A	603	-6.805	21.712	33.306	1.00	28.13	A	N
ATOM	1910	CA	ASP	A	603	-5.913	22.805	33.618	1.00	28.93	A	C
ATOM	1911	CB	ASP	A	603	-5.664	22.865	35.128	1.00	28.98	A	C
ATOM	1912	CG	ASP	A	603	-6.947	23.459	35.987	1.00	33.73	A	C
ATOM	1913	OD1	ASP	A	603	-8.089	23.778	35.443	1.00	28.42	A	O
ATOM	1914	OD2	ASP	A	603	-6.856	23.621	37.282	1.00	35.91	A	O
ATOM	1915	C	ASP	A	603	-4.507	22.701	32.974	1.00	29.04	A	C
ATOM	1916	O	ASP	A	603	-3.891	23.729	32.561	1.00	27.25	A	O
ATOM	1917	N	LEU	A	604	-3.961	21.481	32.975	1.00	27.34	A	N
ATOM	1918	CA	LEU	A	604	-2.652	21.362	32.542	1.00	27.31	A	C
ATOM	1919	CB	LEU	A	604	-2.105	20.048	33.045	1.00	27.86	A	C
ATOM	1920	CG	LEU	A	604	-0.812	19.545	32.431	1.00	25.91	A	C
ATOM	1921	CD1	LEU	A	604	0.205	20.515	32.936	1.00	22.05	A	C

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ATOM	1922	CD2	LEU	A	604	-0.590	17.987	32.747	1.00	20.06	A	C
ATOM	1923	C	LEU	A	604	-2.689	21.458	30.997	1.00	27.94	A	C
ATOM	1924	O	LEU	A	604	-1.713	21.959	30.355	1.00	28.24	A	O
ATOM	1925	N	MET	A	605	-3.812	21.061	30.447	1.00	26.48	A	N
ATOM	1926	CA	MET	A	605	-4.099	21.282	29.067	1.00	28.80	A	C
ATOM	1927	CB	MET	A	605	-5.559	20.852	28.729	1.00	30.62	A	C
ATOM	1928	CG	MET	A	605	-5.769	19.389	28.742	1.00	30.06	A	C
ATOM	1929	SD	MET	A	605	-7.290	18.711	28.035	1.00	28.17	A	S
ATOM	1930	CE	MET	A	605	-7.219	17.156	28.782	1.00	27.94	A	C
ATOM	1931	C	MET	A	605	-3.943	22.800	28.735	1.00	27.74	A	C
ATOM	1932	O	MET	A	605	-3.361	23.201	27.693	1.00	29.19	A	O
ATOM	1933	N	ASN	A	606	-4.450	23.615	29.608	1.00	24.32	A	N
ATOM	1934	CA	ASN	A	606	-4.518	25.008	29.322	1.00	24.85	A	C
ATOM	1935	CB	ASN	A	606	-5.601	25.740	30.143	1.00	22.90	A	C
ATOM	1936	CG	ASN	A	606	-6.956	25.769	29.439	1.00	25.97	A	C
ATOM	1937	OD1	ASN	A	606	-7.104	26.299	28.216	1.00	22.12	A	O
ATOM	1938	ND2	ASN	A	606	-8.008	25.132	30.149	1.00	21.92	A	N
ATOM	1939	C	ASN	A	606	-3.142	25.640	29.448	1.00	24.44	A	C
ATOM	1940	O	ASN	A	606	-2.825	26.484	28.655	1.00	24.24	A	O
ATOM	1941	N	LEU	A	607	-2.364	25.249	30.446	1.00	24.21	A	N
ATOM	1942	CA	LEU	A	607	-0.994	25.656	30.526	1.00	24.98	A	C
ATOM	1943	CB	LEU	A	607	-0.358	24.836	31.553	1.00	25.73	A	C
ATOM	1944	CG	LEU	A	607	-0.020	25.394	32.904	1.00	32.29	A	C
ATOM	1945	CD1	LEU	A	607	1.361	24.815	33.397	1.00	28.44	A	C
ATOM	1946	CD2	LEU	A	607	-0.126	27.011	32.930	1.00	37.04	A	C
ATOM	1947	C	LEU	A	607	-0.242	25.342	29.196	1.00	24.13	A	C
ATOM	1948	O	LEU	A	607	0.447	26.151	28.738	1.00	21.40	A	O
ATOM	1949	N	CYS	A	608	-0.379	24.142	28.643	1.00	24.38	A	N
ATOM	1950	CA	CYS	A	608	0.281	23.770	27.448	1.00	25.94	A	C
ATOM	1951	CB	CYS	A	608	-0.031	22.352	27.043	1.00	26.62	A	C
ATOM	1952	SG	CYS	A	608	0.581	21.098	28.150	1.00	28.65	A	S
ATOM	1953	C	CYS	A	608	-0.153	24.652	26.297	1.00	27.01	A	C
ATOM	1954	O	CYS	A	608	0.618	24.841	25.345	1.00	26.30	A	O
ATOM	1955	N	TRP	A	609	-1.385	25.160	26.379	1.00	27.17	A	N
ATOM	1956	CA	TRP	A	609	-1.912	26.059	25.340	1.00	27.81	A	C
ATOM	1957	CB	TRP	A	609	-3.416	25.793	25.101	1.00	27.37	A	C
ATOM	1958	CG	TRP	A	609	-3.806	24.342	24.755	1.00	26.94	A	C
ATOM	1959	CD1	TRP	A	609	-3.035	23.393	24.086	1.00	25.18	A	C
ATOM	1960	NE1	TRP	A	609	-3.754	22.226	23.939	1.00	25.12	A	N
ATOM	1961	CE2	TRP	A	609	-4.978	22.367	24.527	1.00	25.83	A	C
ATOM	1962	CD2	TRP	A	609	-5.050	23.678	25.068	1.00	24.75	A	C
ATOM	1963	CE3	TRP	A	609	-6.229	24.075	25.689	1.00	20.46	A	C
ATOM	1964	CZ3	TRP	A	609	-7.266	23.194	25.738	1.00	21.37	A	C
ATOM	1965	CH2	TRP	A	609	-7.146	21.865	25.286	1.00	25.28	A	C
ATOM	1966	CZ2	TRP	A	609	-6.026	21.443	24.643	1.00	25.20	A	C
ATOM	1967	C	TRP	A	609	-1.667	27.542	25.722	1.00	28.01	A	C
ATOM	1968	O	TRP	A	609	-2.493	28.470	25.458	1.00	26.64	A	O
ATOM	1969	N	THR	A	610	-0.568	27.773	26.403	1.00	28.14	A	N
ATOM	1970	CA	THR	A	610	-0.154	29.138	26.632	1.00	29.08	A	C
ATOM	1971	CB	THR	A	610	0.968	29.089	27.523	1.00	28.95	A	C
ATOM	1972	OG1	THR	A	610	0.524	28.652	28.814	1.00	26.55	A	O
ATOM	1973	CG2	THR	A	610	1.477	30.465	27.698	1.00	30.70	A	C
ATOM	1974	C	THR	A	610	0.352	29.722	25.292	1.00	28.93	A	C
ATOM	1975	O	THR	A	610	1.329	29.233	24.762	1.00	27.39	A	O
ATOM	1976	N	TYR	A	611	-0.312	30.768	24.794	1.00	29.44	A	N
ATOM	1977	CA	TYR	A	611	-0.072	31.416	23.495	1.00	29.04	A	C
ATOM	1978	CB	TYR	A	611	-1.056	32.600	23.349	1.00	28.96	A	C
ATOM	1979	CG	TYR	A	611	-0.984	33.192	21.986	1.00	27.05	A	C
ATOM	1980	CD1	TYR	A	611	0.050	34.061	21.634	1.00	24.34	A	C
ATOM	1981	CE1	TYR	A	611	0.179	34.517	20.379	1.00	24.28	A	C
ATOM	1982	CZ	TYR	A	611	-0.773	34.124	19.487	1.00	25.90	A	C
ATOM	1983	OH	TYR	A	611	-0.740	34.508	18.266	1.00	26.47	A	O



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ATOM	1984	CE2	TYR	A	611	-1.754	33.248	19.776	1.00	26.03	A	C
ATOM	1985	CD2	TYR	A	611	-1.865	32.794	21.019	1.00	27.40	A	C
ATOM	1986	C	TYR	A	611	1.396	31.810	23.265	1.00	29.55	A	C
ATOM	1987	O	TYR	A	611	2.019	31.420	22.392	1.00	30.80	A	O
ATOM	1988	N	ASP	A	612	1.949	32.633	24.063	1.00	31.35	A	N
ATOM	1989	CA	ASP	A	612	3.351	32.910	24.074	1.00	32.84	A	C
ATOM	1990	CB	ASP	A	612	3.576	34.010	25.068	1.00	33.80	A	C
ATOM	1991	CG	ASP	A	612	4.811	34.799	24.786	1.00	38.36	A	C
ATOM	1992	OD1	ASP	A	612	5.821	34.197	24.363	1.00	42.04	A	O
ATOM	1993	OD2	ASP	A	612	4.886	36.024	24.970	1.00	42.90	A	O
ATOM	1994	C	ASP	A	612	4.315	31.838	24.541	1.00	33.12	A	C
ATOM	1995	O	ASP	A	612	4.514	31.601	25.747	1.00	32.31	A	O
ATOM	1996	N	VAL	A	613	4.953	31.255	23.550	1.00	33.37	A	N
ATOM	1997	CA	VAL	A	613	6.070	30.398	23.673	1.00	35.65	A	C
ATOM	1998	CB	VAL	A	613	6.948	30.724	22.475	1.00	36.55	A	C
ATOM	1999	CG1	VAL	A	613	8.304	30.722	22.757	1.00	36.61	A	C
ATOM	2000	CG2	VAL	A	613	6.641	29.844	21.289	1.00	39.83	A	C
ATOM	2001	C	VAL	A	613	6.843	30.805	24.898	1.00	36.73	A	C
ATOM	2002	O	VAL	A	613	7.295	30.005	25.685	1.00	36.37	A	O
ATOM	2003	N	GLU	A	614	7.021	32.077	25.074	1.00	37.65	A	N
ATOM	2004	CA	GLU	A	614	7.878	32.455	26.152	1.00	39.17	A	C
ATOM	2005	CB	GLU	A	614	8.093	33.978	26.104	1.00	41.32	A	C
ATOM	2006	CG	GLU	A	614	9.527	34.377	26.276	1.00	46.21	A	C
ATOM	2007	CD	GLU	A	614	10.364	34.185	25.014	1.00	49.38	A	C
ATOM	2008	OE1	GLU	A	614	10.145	34.933	23.982	1.00	50.56	A	O
ATOM	2009	OE2	GLU	A	614	11.279	33.330	25.102	1.00	50.25	A	O
ATOM	2010	C	GLU	A	614	7.361	32.051	27.528	1.00	37.63	A	C
ATOM	2011	O	GLU	A	614	8.147	31.751	28.386	1.00	35.68	A	O
ATOM	2012	N	ASN	A	615	6.039	32.017	27.720	1.00	36.76	A	N
ATOM	2013	CA	ASN	A	615	5.513	31.736	29.081	1.00	37.13	A	C
ATOM	2014	CB	ASN	A	615	4.456	32.797	29.486	1.00	38.71	A	C
ATOM	2015	CG	ASN	A	615	5.109	34.220	29.964	1.00	40.40	A	C
ATOM	2016	OD1	ASN	A	615	4.395	35.173	30.134	1.00	43.55	A	O
ATOM	2017	ND2	ASN	A	615	6.424	34.290	30.166	1.00	40.10	A	N
ATOM	2018	C	ASN	A	615	4.945	30.337	29.318	1.00	35.24	A	C
ATOM	2019	O	ASN	A	615	4.426	30.056	30.400	1.00	34.71	A	O
ATOM	2020	N	ARG	A	616	5.142	29.462	28.328	1.00	32.57	A	N
ATOM	2021	CA	ARG	A	616	4.653	28.102	28.320	1.00	32.24	A	C
ATOM	2022	CB	ARG	A	616	4.335	27.704	26.832	1.00	31.24	A	C
ATOM	2023	CG	ARG	A	616	3.742	26.315	26.476	1.00	29.47	A	C
ATOM	2024	CD	ARG	A	616	3.742	25.991	24.803	1.00	22.18	A	C
ATOM	2025	NE	ARG	A	616	3.145	27.089	24.076	1.00	19.84	A	N
ATOM	2026	CZ	ARG	A	616	3.526	27.456	22.862	1.00	21.05	A	C
ATOM	2027	NH1	ARG	A	616	4.436	26.725	22.272	1.00	18.85	A	N
ATOM	2028	NH2	ARG	A	616	3.039	28.557	22.272	1.00	16.86	A	N
ATOM	2029	C	ARG	A	616	5.651	27.177	28.999	1.00	32.27	A	C
ATOM	2030	O	ARG	A	616	6.815	27.159	28.669	1.00	33.97	A	O
ATOM	2031	N	PRO	A	617	5.231	26.352	29.926	1.00	31.84	A	N
ATOM	2032	CA	PRO	A	617	6.203	25.394	30.532	1.00	31.96	A	C
ATOM	2033	CB	PRO	A	617	5.315	24.526	31.477	1.00	29.79	A	C
ATOM	2034	CG	PRO	A	617	4.119	24.564	30.783	1.00	30.46	A	C
ATOM	2035	CD	PRO	A	617	3.853	26.102	30.369	1.00	30.32	A	C
ATOM	2036	C	PRO	A	617	6.810	24.453	29.439	1.00	31.25	A	C
ATOM	2037	O	PRO	A	617	6.248	24.230	28.422	1.00	30.37	A	O
ATOM	2038	N	GLY	A	618	8.021	23.977	29.703	1.00	31.65	A	N
ATOM	2039	CA	GLY	A	618	8.678	22.878	29.043	1.00	29.03	A	C
ATOM	2040	C	GLY	A	618	8.258	21.557	29.681	1.00	28.23	A	C
ATOM	2041	O	GLY	A	618	7.525	21.543	30.717	1.00	27.14	A	O
ATOM	2042	N	PHE	A	619	8.769	20.461	29.129	1.00	26.58	A	N
ATOM	2043	CA	PHE	A	619	8.434	19.108	29.623	1.00	27.51	A	C
ATOM	2044	CB	PHE	A	619	8.764	18.040	28.661	1.00	25.64	A	C
ATOM	2045	CG	PHE	A	619	7.857	17.996	27.455	1.00	26.31	A	C

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ATOM	2046	CD1	PHE	A	619	6.588	17.478	27.542	1.00	23.44	A	C
ATOM	2047	CE1	PHE	A	619	5.734	17.429	26.477	1.00	20.13	A	C
ATOM	2048	CZ	PHE	A	619	6.130	17.805	25.299	1.00	22.28	A	C
ATOM	2049	CE2	PHE	A	619	7.427	18.268	25.111	1.00	24.06	A	C
ATOM	2050	CD2	PHE	A	619	8.277	18.443	26.210	1.00	25.25	A	C
ATOM	2051	C	PHE	A	619	8.983	18.729	31.018	1.00	28.91	A	C
ATOM	2052	O	PHE	A	619	8.340	17.978	31.687	1.00	29.15	A	O
ATOM	2053	N	ALA	A	620	10.101	19.245	31.520	1.00	30.20	A	N
ATOM	2054	CA	ALA	A	620	10.357	18.888	32.925	1.00	32.35	A	C
ATOM	2055	CB	ALA	A	620	11.729	19.407	33.400	1.00	33.10	A	C
ATOM	2056	C	ALA	A	620	9.218	19.481	33.800	1.00	33.42	A	C
ATOM	2057	O	ALA	A	620	8.627	18.781	34.653	1.00	33.54	A	O
ATOM	2058	N	ALA	A	621	8.797	20.717	33.595	1.00	33.03	A	N
ATOM	2059	CA	ALA	A	621	7.666	21.086	34.451	1.00	33.93	A	C
ATOM	2060	CB	ALA	A	621	7.367	22.588	34.348	1.00	32.44	A	C
ATOM	2061	C	ALA	A	621	6.378	20.248	34.241	1.00	34.86	A	C
ATOM	2062	O	ALA	A	621	5.670	19.858	35.191	1.00	36.93	A	O
ATOM	2063	N	VAL	A	622	6.051	19.984	32.984	1.00	33.79	A	N
ATOM	2064	CA	VAL	A	622	4.882	19.235	32.682	1.00	30.94	A	C
ATOM	2065	CB	VAL	A	622	4.763	19.109	31.151	1.00	31.31	A	C
ATOM	2066	CG1	VAL	A	622	3.643	18.127	30.749	1.00	29.12	A	C
ATOM	2067	CG2	VAL	A	622	4.464	20.428	30.530	1.00	30.34	A	C
ATOM	2068	C	VAL	A	622	4.999	17.842	33.200	1.00	30.81	A	C
ATOM	2069	O	VAL	A	622	4.060	17.311	33.732	1.00	29.46	A	O
ATOM	2070	N	GLU	A	623	6.115	17.169	32.942	1.00	30.76	A	N
ATOM	2071	CA	GLU	A	623	6.230	15.796	33.346	1.00	30.65	A	C
ATOM	2072	CB	GLU	A	623	7.547	15.163	32.878	1.00	29.78	A	C
ATOM	2073	CG	GLU	A	623	7.725	13.748	33.436	1.00	29.14	A	C
ATOM	2074	CD	GLU	A	623	8.312	13.621	34.857	1.00	31.26	A	C
ATOM	2075	OE1	GLU	A	623	9.034	14.548	35.354	1.00	30.37	A	O
ATOM	2076	OE2	GLU	A	623	8.118	12.533	35.470	1.00	29.40	A	O
ATOM	2077	C	GLU	A	623	6.106	15.752	34.851	1.00	31.83	A	C
ATOM	2078	O	GLU	A	623	5.437	14.916	35.363	1.00	30.64	A	O
ATOM	2079	N	LEU	A	624	6.719	16.676	35.560	1.00	34.13	A	N
ATOM	2080	CA	LEU	A	624	6.629	16.690	37.037	1.00	36.85	A	C
ATOM	2081	CB	LEU	A	624	7.552	17.812	37.626	1.00	38.21	A	C
ATOM	2082	CG	LEU	A	624	7.495	18.010	39.152	1.00	43.27	A	C
ATOM	2083	CD1	LEU	A	624	8.021	16.714	39.868	1.00	42.63	A	C
ATOM	2084	CD2	LEU	A	624	8.291	19.321	39.609	1.00	44.35	A	C
ATOM	2085	C	LEU	A	624	5.206	16.822	37.594	1.00	37.05	A	C
ATOM	2086	O	LEU	A	624	4.796	16.285	38.660	1.00	36.69	A	O
ATOM	2087	N	ARG	A	625	4.453	17.603	36.879	1.00	37.58	A	N
ATOM	2088	CA	ARG	A	625	3.087	17.850	37.251	1.00	38.06	A	C
ATOM	2089	CB	ARG	A	625	2.531	18.843	36.263	1.00	39.86	A	C
ATOM	2090	CG	ARG	A	625	1.225	19.341	36.686	1.00	45.14	A	C
ATOM	2091	CD	ARG	A	625	1.357	20.461	37.638	1.00	51.11	A	C
ATOM	2092	NE	ARG	A	625	0.323	21.363	37.253	1.00	53.02	A	N
ATOM	2093	CZ	ARG	A	625	0.455	22.640	37.018	1.00	51.22	A	C
ATOM	2094	NH1	ARG	A	625	1.625	23.267	37.194	1.00	50.98	A	N
ATOM	2095	NH2	ARG	A	625	-0.641	23.260	36.601	1.00	48.82	A	N
ATOM	2096	C	ARG	A	625	2.249	16.612	37.082	1.00	37.76	A	C
ATOM	2097	O	ARG	A	625	1.278	16.288	37.914	1.00	38.59	A	O
ATOM	2098	N	LEU	A	626	2.556	15.917	35.990	1.00	33.69	A	N
ATOM	2099	CA	LEU	A	626	1.714	14.876	35.626	1.00	30.77	A	C
ATOM	2100	CB	LEU	A	626	2.049	14.355	34.238	1.00	30.21	A	C
ATOM	2101	CG	LEU	A	626	1.049	14.840	33.303	1.00	29.80	A	C
ATOM	2102	CD1	LEU	A	626	1.477	14.491	31.954	1.00	28.00	A	C
ATOM	2103	CD2	LEU	A	626	-0.224	14.239	33.724	1.00	28.84	A	C
ATOM	2104	C	LEU	A	626	2.079	13.829	36.577	1.00	30.31	A	C
ATOM	2105	O	LEU	A	626	1.207	13.147	37.013	1.00	29.37	A	O
ATOM	2106	N	ARG	A	627	3.379	13.602	36.768	1.00	30.12	A	N
ATOM	2107	CA	ARG	A	627	3.826	12.590	37.699	1.00	32.08	A	C

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ATOM	2108	CB	ARG	A	627	5.320	12.680	37.915	1.00	33.23	A	C
ATOM	2109	CG	ARG	A	627	5.825	11.509	38.759	1.00	32.95	A	C
ATOM	2110	CD	ARG	A	627	7.182	11.784	39.305	1.00	36.79	A	C
ATOM	2111	NE	ARG	A	627	8.032	12.636	38.464	1.00	38.66	A	N
ATOM	2112	CZ	ARG	A	627	9.137	13.303	38.893	1.00	40.75	A	C
ATOM	2113	NH1	ARG	A	627	9.533	13.283	40.243	1.00	41.93	A	N
ATOM	2114	NH2	ARG	A	627	9.802	14.052	37.992	1.00	35.61	A	N
ATOM	2115	C	ARG	A	627	3.242	12.813	39.110	1.00	32.18	A	C
ATOM	2116	O	ARG	A	627	2.698	11.915	39.690	1.00	31.30	A	O
ATOM	2117	N	ASN	A	628	3.285	14.032	39.636	1.00	33.12	A	N
ATOM	2118	CA	ASN	A	628	2.786	14.231	41.010	1.00	33.28	A	C
ATOM	2119	CB	ASN	A	628	3.088	15.634	41.495	1.00	33.21	A	C
ATOM	2120	CG	ASN	A	628	4.580	15.826	41.840	1.00	32.39	A	C
ATOM	2121	OD1	ASN	A	628	5.341	14.869	41.941	1.00	28.19	A	O
ATOM	2122	ND2	ASN	A	628	4.986	17.061	42.004	1.00	34.21	A	N
ATOM	2123	C	ASN	A	628	1.324	13.937	41.119	1.00	33.87	A	C
ATOM	2124	O	ASN	A	628	0.875	13.337	42.070	1.00	35.12	A	O
ATOM	2125	N	TYR	A	629	0.568	14.228	40.062	1.00	33.75	A	N
ATOM	2126	CA	TYR	A	629	-0.856	14.030	40.154	1.00	32.19	A	C
ATOM	2127	CB	TYR	A	629	-1.577	14.938	39.176	1.00	32.45	A	C
ATOM	2128	CG	TYR	A	629	-3.037	14.696	39.057	1.00	34.61	A	C
ATOM	2129	CD1	TYR	A	629	-3.944	15.153	40.089	1.00	33.77	A	C
ATOM	2130	CE1	TYR	A	629	-5.300	14.954	39.983	1.00	31.14	A	C
ATOM	2131	CZ	TYR	A	629	-5.769	14.280	38.888	1.00	30.88	A	C
ATOM	2132	OH	TYR	A	629	-7.090	14.056	38.822	1.00	34.84	A	O
ATOM	2133	CE2	TYR	A	629	-4.950	13.809	37.866	1.00	32.73	A	C
ATOM	2134	CD2	TYR	A	629	-3.568	14.056	37.927	1.00	33.97	A	C
ATOM	2135	C	TYR	A	629	-1.083	12.567	39.978	1.00	32.25	A	C
ATOM	2136	O	TYR	A	629	-1.994	11.919	40.579	1.00	34.10	A	O
ATOM	2137	N	TYR	A	630	-0.241	11.925	39.205	1.00	30.69	A	N
ATOM	2138	CA	TYR	A	630	-0.558	10.529	39.035	1.00	29.66	A	C
ATOM	2139	CB	TYR	A	630	0.331	9.941	37.988	1.00	28.03	A	C
ATOM	2140	CG	TYR	A	630	0.208	8.436	37.831	1.00	28.13	A	C
ATOM	2141	CD1	TYR	A	630	-0.979	7.843	37.418	1.00	30.09	A	C
ATOM	2142	CE1	TYR	A	630	-1.071	6.417	37.253	1.00	28.70	A	C
ATOM	2143	CZ	TYR	A	630	0.010	5.629	37.559	1.00	28.94	A	C
ATOM	2144	OH	TYR	A	630	-0.073	4.276	37.410	1.00	33.75	A	O
ATOM	2145	CE2	TYR	A	630	1.165	6.174	38.021	1.00	28.80	A	C
ATOM	2146	CD2	TYR	A	630	1.265	7.605	38.108	1.00	28.96	A	C
ATOM	2147	C	TYR	A	630	-0.298	9.799	40.370	1.00	29.50	A	C
ATOM	2148	O	TYR	A	630	-1.020	8.959	40.824	1.00	24.81	A	O
ATOM	2149	N	TYR	A	631	0.868	9.996	40.872	1.00	32.27	A	N
ATOM	2150	CA	TYR	A	631	1.110	9.392	42.169	1.00	36.87	A	C
ATOM	2151	CB	TYR	A	631	2.585	9.491	42.624	1.00	38.07	A	C
ATOM	2152	CG	TYR	A	631	3.388	8.605	41.696	1.00	41.33	A	C
ATOM	2153	CD1	TYR	A	631	2.881	7.342	41.331	1.00	42.71	A	C
ATOM	2154	CE1	TYR	A	631	3.591	6.481	40.485	1.00	44.48	A	C
ATOM	2155	CZ	TYR	A	631	4.828	6.869	39.953	1.00	46.30	A	C
ATOM	2156	OH	TYR	A	631	5.479	5.996	39.093	1.00	45.56	A	O
ATOM	2157	CE2	TYR	A	631	5.375	8.122	40.302	1.00	46.01	A	C
ATOM	2158	CD2	TYR	A	631	4.632	8.996	41.186	1.00	44.01	A	C
ATOM	2159	C	TYR	A	631	0.108	9.863	43.170	1.00	37.15	A	C
ATOM	2160	O	TYR	A	631	-0.293	9.106	43.903	1.00	36.51	A	O
ATOM	2161	N	ASP	A	632	-0.385	11.070	43.088	1.00	40.04	A	N
ATOM	2162	CA	ASP	A	632	-1.427	11.440	43.989	1.00	44.79	A	C
ATOM	2163	CB	ASP	A	632	-1.812	12.906	43.724	1.00	47.43	A	C
ATOM	2164	CG	ASP	A	632	-1.527	13.801	44.928	1.00	52.14	A	C
ATOM	2165	OD1	ASP	A	632	-2.204	13.470	45.989	1.00	57.92	A	O
ATOM	2166	OD2	ASP	A	632	-0.677	14.778	44.913	1.00	47.50	A	O
ATOM	2167	C	ASP	A	632	-2.645	10.519	43.821	1.00	46.10	A	C
ATOM	2168	O	ASP	A	632	-3.330	10.139	44.790	1.00	46.49	A	O
ATOM	2169	N	VAL	A	633	-2.924	10.141	42.575	1.00	46.54	A	N

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ATOM	2170	CA	VAL	A	633	-4.099	9.363	42.305	1.00	45.81	A	C
ATOM	2171	CB	VAL	A	633	-4.398	9.340	40.754	1.00	45.98	A	C
ATOM	2172	CG1	VAL	A	633	-5.306	8.249	40.452	1.00	44.50	A	C
ATOM	2173	CG2	VAL	A	633	-5.130	10.608	40.336	1.00	45.06	A	C
ATOM	2174	C	VAL	A	633	-3.958	7.976	42.850	1.00	46.18	A	C
ATOM	2175	O	VAL	A	633	-4.935	7.370	43.295	1.00	44.74	A	O
ATOM	2176	N	VAL	A	634	-2.748	7.435	42.771	1.00	47.30	A	N
ATOM	2177	CA	VAL	A	634	-2.531	6.108	43.294	1.00	48.89	A	C
ATOM	2178	CB	VAL	A	634	-1.182	5.574	42.913	1.00	49.28	A	C
ATOM	2179	CG1	VAL	A	634	-0.942	5.671	41.395	1.00	49.29	A	C
ATOM	2180	CG2	VAL	A	634	-0.167	6.354	43.626	1.00	50.64	A	C
ATOM	2181	C	VAL	A	634	-2.576	6.148	44.844	1.00	49.69	A	C
ATOM	2229	O1A	ANP	B	1	3.564	5.579	9.725	1.00	54.29	B	O
ATOM	2230	PA	ANP	B	1	2.948	5.871	11.026	1.00	48.36	B	P
ATOM	2231	O2A	ANP	B	1	4.090	5.969	11.929	1.00	39.73	B	O
ATOM	2232	O3A	ANP	B	1	2.184	7.080	10.521	1.00	53.40	B	O
ATOM	2233	PB	ANP	B	1	2.377	7.430	9.059	1.00	51.91	B	P
ATOM	2234	O1B	ANP	B	1	3.640	6.839	8.735	1.00	48.88	B	O
ATOM	2235	O2B	ANP	B	1	2.736	8.899	9.149	1.00	52.17	B	O
ATOM	2236	N3B	ANP	B	1	1.360	6.817	7.915	1.00	59.86	B	N
ATOM	2237	PG	ANP	B	1	-0.321	6.754	8.244	1.00	70.46	B	P
ATOM	2238	O3G	ANP	B	1	-1.060	7.802	7.399	1.00	68.96	B	O
ATOM	2239	O2G	ANP	B	1	-0.472	6.940	9.776	1.00	71.23	B	O
ATOM	2240	O1G	ANP	B	1	-0.959	5.482	7.728	1.00	70.14	B	O
ATOM	2241	O5*	ANP	B	1	1.905	4.862	11.178	1.00	47.63	B	O
ATOM	2242	C5*	ANP	B	1	1.765	3.689	10.396	1.00	48.17	B	C
ATOM	2243	C4*	ANP	B	1	0.919	2.622	11.150	1.00	46.18	B	C
ATOM	2244	O4*	ANP	B	1	1.688	1.439	11.318	1.00	42.54	B	O
ATOM	2245	C1*	ANP	B	1	1.697	0.924	12.597	1.00	40.62	B	C
ATOM	2246	C2*	ANP	B	1	0.614	1.739	13.301	1.00	44.89	B	C
ATOM	2247	O2*	ANP	B	1	-0.671	1.120	13.025	1.00	44.16	B	O
ATOM	2248	C3*	ANP	B	1	0.599	3.058	12.579	1.00	45.39	B	C
ATOM	2249	O3*	ANP	B	1	-0.626	3.776	12.802	1.00	45.80	B	O
ATOM	2250	N9	ANP	B	1	3.052	0.994	13.167	1.00	32.97	B	N
ATOM	2251	C8	ANP	B	1	4.101	1.692	12.757	1.00	33.03	B	C
ATOM	2252	N7	ANP	B	1	5.202	1.397	13.565	1.00	31.49	B	N
ATOM	2253	C5	ANP	B	1	4.844	0.482	14.432	1.00	30.44	B	C
ATOM	2254	C6	ANP	B	1	5.420	-0.180	15.600	1.00	30.81	B	C
ATOM	2255	N6	ANP	B	1	6.765	0.070	15.890	1.00	27.10	B	N
ATOM	2256	C4	ANP	B	1	3.455	0.227	14.165	1.00	30.83	B	C
ATOM	2257	N3	ANP	B	1	2.839	-0.624	14.961	1.00	27.60	B	N
ATOM	2258	C2	ANP	B	1	3.442	-1.255	15.976	1.00	27.45	B	C
ATOM	2259	N1	ANP	B	1	4.688	-1.105	16.309	1.00	27.69	B	N
ATOM	2185	N	VAL	C	1	-6.369	15.938	8.091	1.00	54.58	C	N
ATOM	2186	CA	VAL	C	1	-5.350	16.083	9.198	1.00	55.94	C	C
ATOM	2187	CB	VAL	C	1	-5.105	14.788	10.002	1.00	56.18	C	C
ATOM	2188	CG1	VAL	C	1	-5.747	13.589	9.372	1.00	56.39	C	C
ATOM	2189	CG2	VAL	C	1	-3.607	14.556	10.216	1.00	56.90	C	C
ATOM	2190	C	VAL	C	1	-3.945	16.624	8.826	1.00	55.80	C	C
ATOM	2191	O	VAL	C	1	-3.252	17.179	9.660	1.00	54.81	C	O
ATOM	2192	N	TYR	C	2	-3.499	16.451	7.601	0.70	55.59	C	N
ATOM	2193	CA	TYR	C	2	-2.220	17.038	7.311	0.70	55.46	C	C
ATOM	2194	CB	TYR	C	2	-1.251	15.999	6.821	0.70	54.01	C	C
ATOM	2195	CG	TYR	C	2	-0.592	15.199	7.904	0.70	48.77	C	C
ATOM	2196	CD1	TYR	C	2	0.450	15.719	8.625	0.70	44.38	C	C
ATOM	2197	CE1	TYR	C	2	1.060	14.994	9.606	0.70	42.29	C	C
ATOM	2198	CZ	TYR	C	2	0.659	13.739	9.857	0.70	41.35	C	C
ATOM	2199	OH	TYR	C	2	1.316	13.053	10.800	0.70	39.82	C	O
ATOM	2200	CE2	TYR	C	2	-0.358	13.175	9.139	0.70	42.47	C	C
ATOM	2201	CD2	TYR	C	2	-0.976	13.901	8.166	0.70	44.80	C	C
ATOM	2202	C	TYR	C	2	-2.514	18.041	6.255	0.70	57.02	C	C
ATOM	2203	O	TYR	C	2	-2.796	17.662	5.141	0.70	56.09	C	O

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ATOM	2204	N	ASP	C	3	-2.492	19.321	6.627	0.70	59.68	C	N
ATOM	2205	CA	ASP	C	3	-2.844	20.412	5.700	0.70	62.18	C	C
ATOM	2206	CB	ASP	C	3	-3.553	21.638	6.381	0.70	61.64	C	C
ATOM	2207	CG	ASP	C	3	-4.908	21.286	7.098	0.70	62.33	C	C
ATOM	2208	OD1	ASP	C	3	-5.767	22.199	7.344	0.70	58.88	C	O
ATOM	2209	OD2	ASP	C	3	-5.198	20.136	7.515	0.70	64.32	C	O
ATOM	2210	C	ASP	C	3	-1.562	20.851	4.990	0.70	63.79	C	C
ATOM	2211	O	ASP	C	3	-0.619	21.328	5.628	0.70	63.18	C	O
ATOM	2212	N	ASP	C	4	-1.538	20.649	3.674	0.60	66.36	C	N
ATOM	2213	CA	ASP	C	4	-0.422	21.075	2.823	0.60	69.26	C	C
ATOM	2214	CB	ASP	C	4	-0.336	20.239	1.526	0.60	70.03	C	C
ATOM	2215	CG	ASP	C	4	0.177	18.808	1.750	0.60	71.71	C	C
ATOM	2216	OD1	ASP	C	4	-0.654	17.862	1.785	0.60	71.91	C	O
ATOM	2217	OD2	ASP	C	4	1.401	18.532	1.863	0.60	72.94	C	O
ATOM	2218	C	ASP	C	4	-0.700	22.492	2.400	0.60	70.38	C	C
ATOM	2219	O	ASP	C	4	-1.864	22.852	2.256	0.60	70.35	C	O
ATOM	2220	N	GLU	C	5	0.341	23.294	2.170	0.60	71.94	C	N
ATOM	2221	CA	GLU	C	5	0.111	24.643	1.617	0.60	73.22	C	C
ATOM	2222	CB	GLU	C	5	0.913	25.699	2.362	0.60	73.92	C	C
ATOM	2223	CG	GLU	C	5	0.046	26.871	2.827	0.60	76.02	C	C
ATOM	2224	CD	GLU	C	5	0.879	28.028	3.353	0.60	78.11	C	C
ATOM	2225	OE1	GLU	C	5	0.332	28.870	4.102	0.60	78.84	C	O
ATOM	2226	OE2	GLU	C	5	2.078	28.099	3.003	0.60	79.08	C	O
ATOM	2227	C	GLU	C	5	0.293	24.777	0.081	0.60	72.97	C	C
ATOM	2228	O	GLU	C	5	1.250	24.261	-0.517	0.60	72.49	C	O
ATOM	2260	MG	MG	M	1	1.874	8.821	11.823	1.00	36.22	M	MG
ATOM	2261	MG	Mg	M	2	5.113	9.347	7.280	1.00	42.44	M	MG
ATOM	2262	O	HOH	W	1	4.396	18.403	17.714	0.70	15.89	W	O
ATOM	2263	O	HOH	W	2	3.499	22.603	18.031	1.00	32.99	W	O
ATOM	2264	O	HOH	W	3	14.308	4.378	22.865	1.00	28.04	W	O
ATOM	2265	O	HOH	W	4	-1.893	34.009	16.353	1.00	28.18	W	O
ATOM	2266	O	HOH	W	5	-5.001	27.854	27.241	1.00	29.99	W	O
ATOM	2267	O	HOH	W	6	-13.428	18.613	18.577	1.00	38.09	W	O
ATOM	2268	O	HOH	W	7	-7.565	24.107	22.534	1.00	26.65	W	O
ATOM	2269	O	HOH	W	8	10.503	22.874	32.408	0.50	10.92	W	O
ATOM	2270	O	HOH	W	9	-9.786	6.235	37.368	1.00	30.76	W	O
ATOM	2271	O	HOH	W	10	12.089	11.259	30.963	1.00	29.63	W	O
ATOM	2272	O	HOH	W	11	7.754	13.383	13.053	1.00	38.77	W	O
ATOM	2273	O	HOH	W	12	-4.215	11.841	16.489	1.00	24.06	W	O
ATOM	2274	O	HOH	W	13	-7.189	25.748	7.217	1.00	50.85	W	O
ATOM	2275	O	HOH	W	14	-4.418	30.412	26.587	1.00	33.52	W	O
ATOM	2276	O	HOH	W	15	9.238	25.095	32.187	0.70	15.59	W	O
ATOM	2277	O	HOH	W	16	-2.559	31.515	26.343	1.00	32.13	W	O
ATOM	2278	O	HOH	W	17	-3.647	28.453	9.823	1.00	29.49	W	O
ATOM	2279	O	HOH	W	18	-5.535	-2.478	20.147	1.00	29.90	W	O
ATOM	2280	O	HOH	W	19	17.125	7.862	28.531	1.00	31.52	W	O
ATOM	2281	O	HOH	W	20	-4.496	0.480	18.361	1.00	28.11	W	O
ATOM	2282	O	HOH	W	21	10.459	16.951	35.365	1.00	24.45	W	O
ATOM	2283	O	HOH	W	22	-4.933	12.027	13.915	1.00	23.36	W	O
ATOM	2284	O	HOH	W	23	-10.946	24.266	37.615	1.00	51.98	W	O
ATOM	2285	O	HOH	W	24	-3.938	23.425	18.581	1.00	24.96	W	O
ATOM	2286	O	HOH	W	25	-10.034	17.642	13.381	1.00	25.08	W	O
ATOM	2287	O	HOH	W	26	5.663	20.814	16.866	0.30	8.89	W	O
ATOM	2288	O	HOH	W	27	13.690	23.612	22.535	1.00	33.54	W	O
ATOM	2289	O	HOH	W	28	25.926	12.104	16.347	0.50	23.45	W	O
ATOM	2290	O	HOH	W	29	-8.326	25.770	33.031	1.00	37.37	W	O
ATOM	2291	O	HOH	W	30	-2.770	2.681	35.609	1.00	46.80	W	O
ATOM	2292	O	HOH	W	31	-15.876	14.638	25.854	1.00	35.92	W	O
ATOM	2293	O	HOH	W	32	4.317	31.993	20.936	1.00	29.00	W	O
ATOM	2294	O	HOH	W	33	17.396	16.400	11.734	1.00	41.98	W	O
ATOM	2295	O	HOH	W	34	11.936	22.036	30.142	1.00	24.90	W	O
ATOM	2296	O	HOH	W	35	23.503	33.428	17.782	1.00	46.46	W	O

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ATOM	2297	O	HOH	W	36	26.670	-5.080	7.409	1.00	40.16	W	O
ATOM	2298	O	HOH	W	37	5.534	21.977	37.255	1.00	42.10	W	O
ATOM	2299	O	HOH	W	38	21.763	12.593	34.964	1.00	41.54	W	O
ATOM	2300	O	HOH	W	39	12.530	8.771	30.979	1.00	24.15	W	O
ATOM	2301	O	HOH	W	40	11.265	-12.613	5.730	1.00	44.86	W	O
ATOM	2302	O	HOH	W	41	-4.664	33.223	23.276	1.00	24.68	W	O
ATOM	2303	O	HOH	W	42	-0.982	8.388	49.268	1.00	37.25	W	O
ATOM	2304	O	HOH	W	43	2.943	5.992	14.434	1.00	31.06	W	O
ATOM	2305	O	HOH	W	44	9.447	-7.361	1.156	1.00	52.68	W	O
ATOM	2306	O	HOH	W	45	-0.446	-0.636	15.143	1.00	29.21	W	O
ATOM	2307	O	HOH	W	46	10.821	21.456	4.398	1.00	36.61	W	O
ATOM	2308	O	HOH	W	47	0.847	34.046	26.512	1.00	28.07	W	O
ATOM	2309	O	HOH	W	48	5.443	12.542	10.741	1.00	32.09	W	O
ATOM	2310	O	HOH	W	49	5.545	11.508	6.845	1.00	34.17	W	O
ATOM	2311	O	HOH	W	50	-14.457	16.336	24.440	1.00	30.73	W	O
ATOM	2312	O	HOH	W	51	-13.495	17.322	11.396	1.00	39.66	W	O
ATOM	2313	O	HOH	W	52	-6.503	31.977	10.316	1.00	48.95	W	O
ATOM	2314	O	HOH	W	53	-7.007	-4.910	24.927	1.00	46.61	W	O
ATOM	2315	O	HOH	W	54	24.699	18.618	24.789	1.00	34.18	W	O
ATOM	2316	O	HOH	W	55	-1.626	30.216	33.608	1.00	57.60	W	O
ATOM	2317	O	HOH	W	56	-8.764	39.152	22.861	1.00	52.23	W	O
ATOM	2318	O	HOH	W	57	25.214	13.766	15.773	0.50	22.95	W	O
ATOM	2319	O	HOH	W	58	17.280	2.912	20.594	1.00	39.47	W	O
ATOM	2320	O	HOH	W	59	-8.157	24.987	38.958	1.00	33.69	W	O
ATOM	2321	O	HOH	W	60	-9.481	36.577	25.236	1.00	40.51	W	O
ATOM	2322	O	HOH	W	61	-16.156	22.524	28.123	1.00	29.33	W	O
ATOM	2323	O	HOH	W	62	-3.079	24.788	16.098	1.00	29.98	W	O
ATOM	2324	O	HOH	W	63	6.496	3.480	37.308	1.00	41.16	W	O
ATOM	2325	O	HOH	W	64	-11.981	11.954	30.541	1.00	38.47	W	O
ATOM	2326	O	HOH	W	65	16.670	10.043	30.808	1.00	38.06	W	O
ATOM	2327	O	HOH	W	66	0.039	30.083	31.237	1.00	44.09	W	O
ATOM	2328	O	HOH	W	67	29.285	-5.425	6.851	1.00	48.32	W	O
ATOM	2329	O	HOH	W	68	11.926	24.443	24.122	1.00	39.11	W	O
ATOM	2330	O	HOH	W	69	16.581	25.720	11.850	1.00	38.40	W	O
ATOM	2331	O	HOH	W	70	-12.698	6.800	35.171	1.00	24.27	W	O
ATOM	2332	O	HOH	W	71	22.068	10.599	32.933	1.00	43.56	W	O
ATOM	2333	O	HOH	W	72	-16.537	9.030	29.746	1.00	40.14	W	O
ATOM	2334	O	HOH	W	73	26.599	3.416	12.246	1.00	41.92	W	O
ATOM	2335	O	HOH	W	74	2.898	-2.865	30.508	1.00	29.16	W	O
ATOM	2336	O	HOH	W	75	19.251	9.611	34.117	1.00	50.34	W	O
ATOM	2337	O	HOH	W	76	-11.751	9.897	37.706	1.00	39.00	W	O
ATOM	2338	O	HOH	W	77	13.271	34.762	6.569	1.00	52.68	W	O
ATOM	2339	O	HOH	W	78	26.070	-5.560	4.943	1.00	35.20	W	O
ATOM	2340	O	HOH	W	79	14.131	0.840	27.112	1.00	42.65	W	O
ATOM	2341	O	HOH	W	80	8.534	25.524	34.270	0.30	9.69	W	O
ATOM	2342	O	HOH	W	81	27.097	-3.545	2.962	1.00	49.98	W	O
ATOM	2343	O	HOH	W	82	23.358	33.250	15.224	1.00	47.88	W	O
ATOM	2344	O	HOH	W	83	6.802	2.847	34.417	1.00	50.11	W	O
ATOM	2345	O	HOH	W	84	-3.157	29.882	28.878	1.00	42.35	W	O
ATOM	2346	O	HOH	W	85	2.243	2.850	36.647	1.00	45.56	W	O
ATOM	2347	O	HOH	W	86	-3.401	16.590	46.388	1.00	54.03	W	O
ATOM	2348	O	HOH	W	87	-10.648	30.380	8.157	1.00	35.80	W	O
ATOM	2349	O	HOH	W	88	8.515	5.435	42.151	1.00	47.29	W	O
ATOM	2350	O	HOH	W	89	6.221	6.449	36.848	1.00	35.73	W	O
ATOM	2351	O	HOH	W	90	13.922	14.921	37.200	1.00	39.84	W	O
ATOM	2352	O	HOH	W	91	20.768	10.478	28.348	1.00	50.37	W	O
ATOM	2353	O	HOH	W	92	-3.949	26.248	33.690	1.00	30.18	W	O
ATOM	2354	O	HOH	W	93	23.298	26.350	7.080	1.00	54.47	W	O
ATOM	2355	O	HOH	W	94	5.721	28.372	32.345	1.00	48.90	W	O
ATOM	2356	O	HOH	W	95	26.475	30.211	14.259	1.00	37.37	W	O
ATOM	2357	O	HOH	W	96	19.698	8.609	28.358	1.00	35.06	W	O
ATOM	2358	O	HOH	W	97	25.527	31.710	16.988	1.00	50.19	W	O

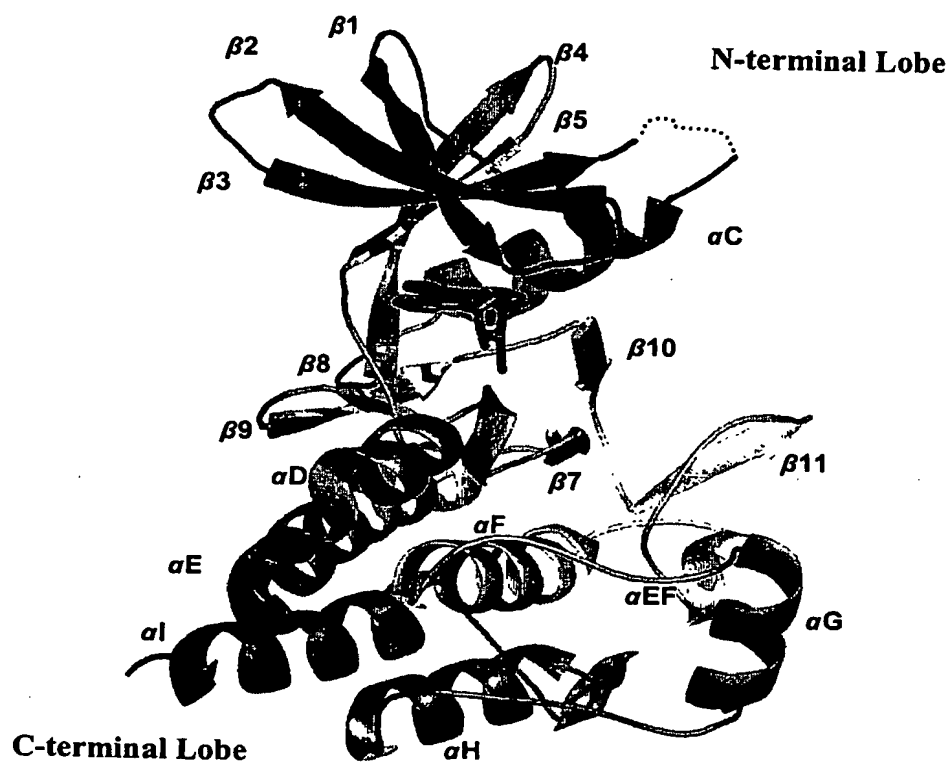
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Figure 2A - 39

ATOM	2359	O	HOH	W	98	0.790	33.861	29.429	1.00	41.93	W	O
END												

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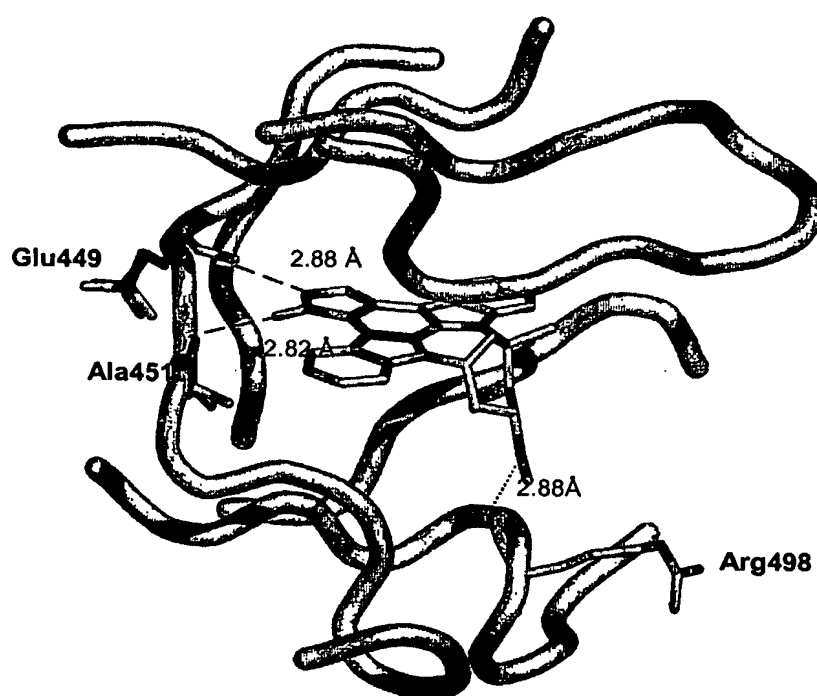
Figure 3





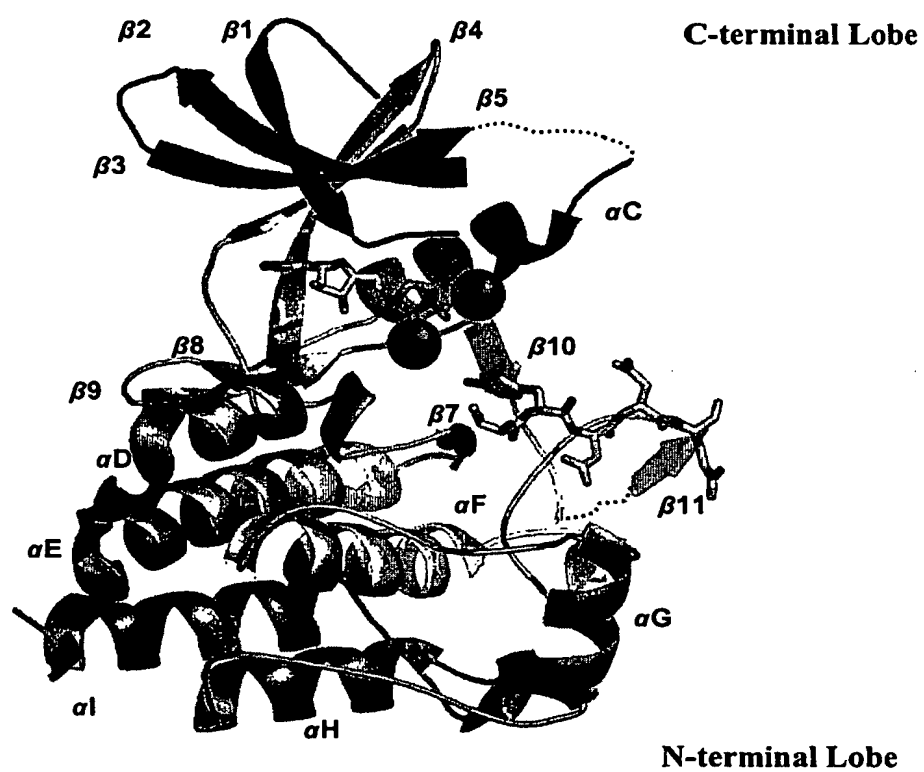
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Figure 4



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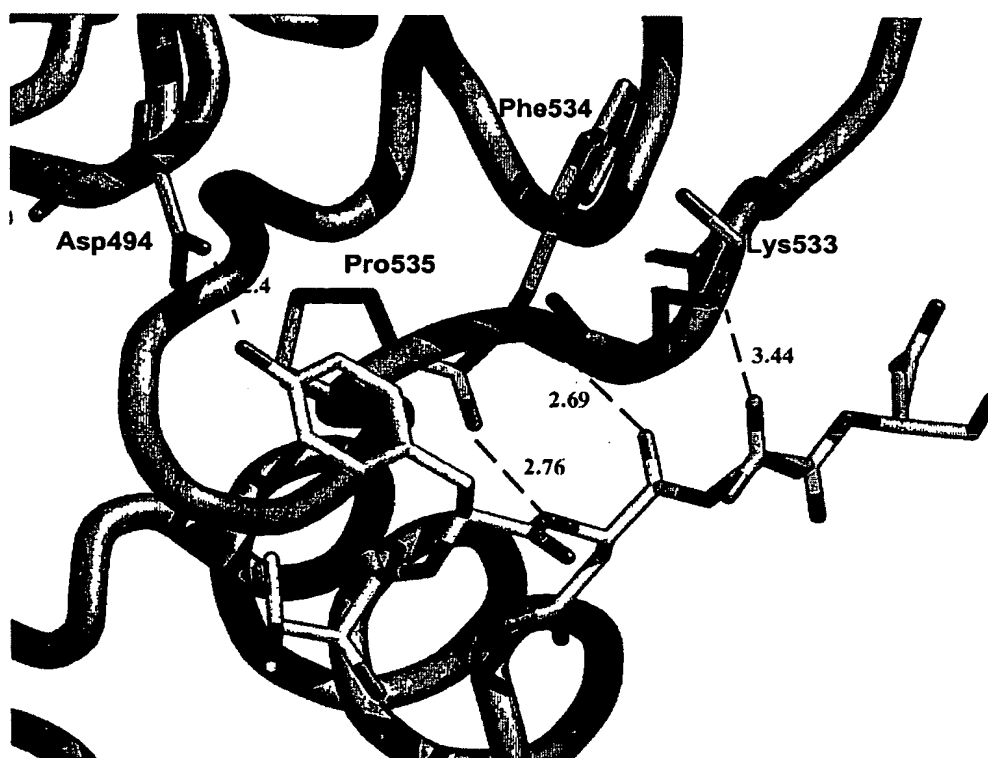
Figure 5



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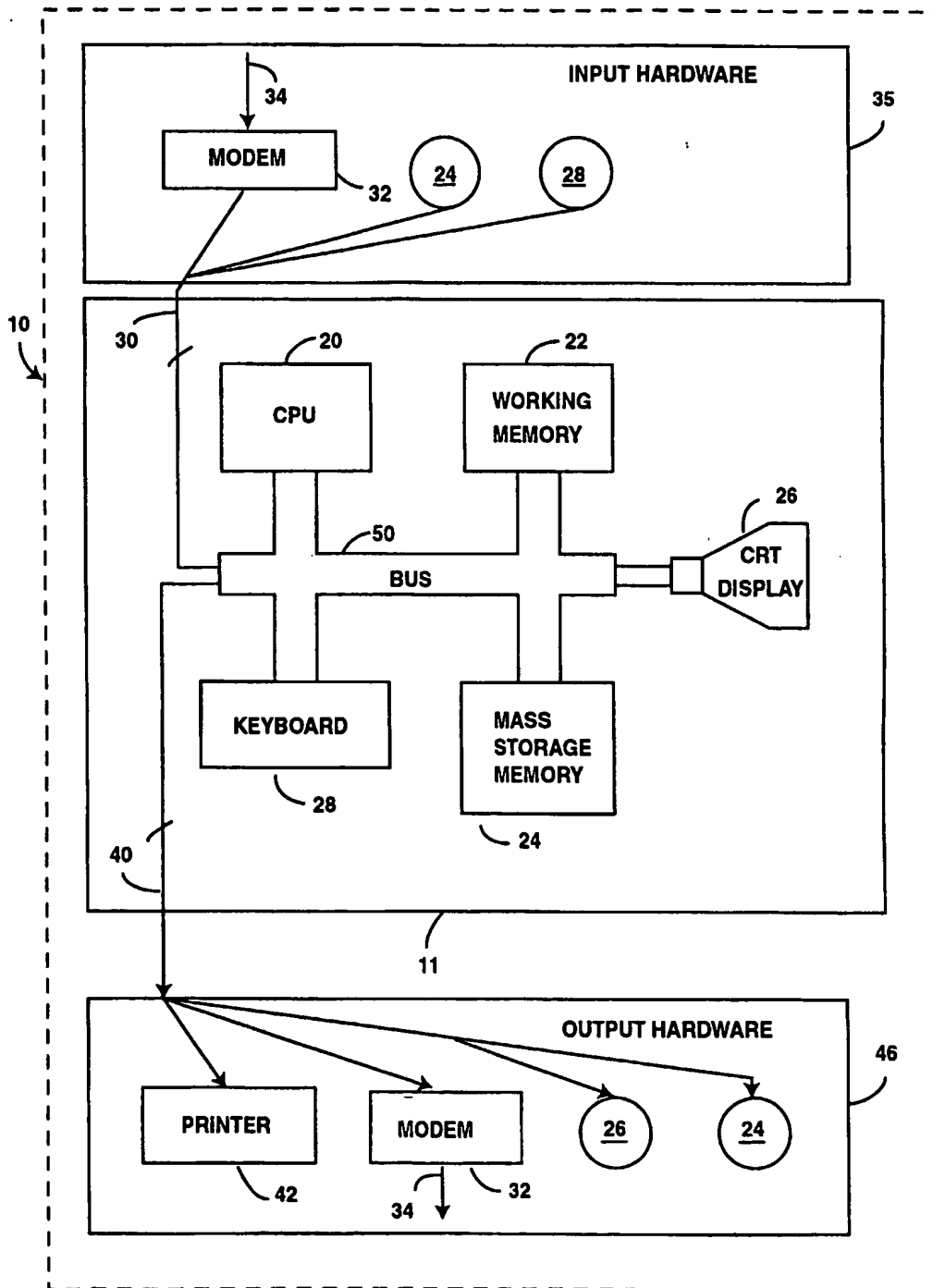
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Figure 6



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Figure 7



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Figure 8

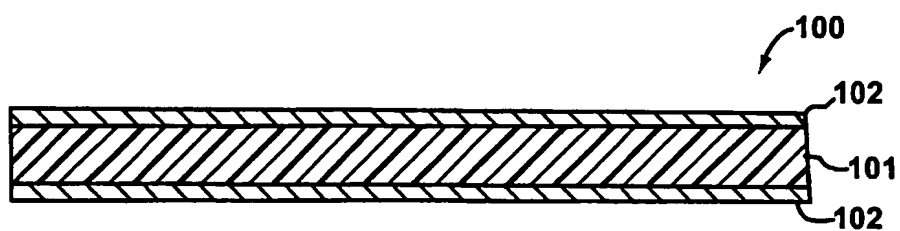


Figure 9

